Chemical **C**ompound **D**eep **D**ata **S**ource

Deep Complementary Data Sheet

(A Sample DCDS: Constant Property Example)

Normal Boiling Point of (2R)-2-Methylcyclohexan-1-one

DCDS-PC22-CT1001897301-ed1-2022

February 2022

How to Order DCDS

ChemEssen, Inc.

About DCDS

Deep Complementary Data Sheet (DCDS) provides the property data of both target chemical compound and similar compounds to assist your in-depth analysis for the case when the reliability of a specific property value of your target chemical compound becomes important.

The data categories covered by DCDS are constant and temperature dependent thermo-physicochemical, thermodynamic, transport, and pharmaceutical properties listed on the Deep Data list page.

DCDS provides the property data determined based on (1) QSQN technology, (2) QN technology if applicable, (3) the existing estimation methods if applicable, and (4) the experimental data with reference and the refined experimental data if available.

Chances to secure a reliable range of the target property value may become much higher by analyzing the experimental data, computational data, and the trend of the data for both the target compound and similar compounds. An example of the analysis is given in the "Data Quality Inspection" section of the QSQN technology description page.

About QSQN & QN Technologies

The 41 patented QSQN technology is based on the combination of quantum chemistry, statistical thermodynamics, 3D QSPR (Quantitative Structure–Property Relationships), and neural network in conjunction with a systematic analysis of the experimental data available to date. It has been commercialized as an online chemical database named Mol-Instincts, which provides more than 2,000 datasets per single chemical compound. It has been cited a number of times in the scientific publications of high-impact journals including NATURE, ELSEVIER, Springer, American Chemical Society, Royal Society of Chemistry, and Wiley. More than 490,000 individuals, 1,400 universities, 300 global companies, and 100 national organizations around the world have used Mol-Instincts.

The QN technology consists of 2D QSPR and neural network without quantum computations to be able to produce the property data in real-time. It has been commercialized as a webservice called ChemRTP, which provides more than 25 important properties of chemical compounds in real-time for any compound consisting of C, H, N, O, S, F, Cl, Br, I, Si, P, and/or As atoms.

Please refer to the technology description page for more details on QSQN and QN technologies.

How to Cite This DCDS

Normal Boiling Point of (2R)-2-Methylcyclohexan-1-one, Deep Complementary Data Sheet (DCDS), No. DCDS-PC22-CT1001897301-ed1-2022, CCDDS (Chemical Compound Deep Data Source; https://www.molinstincts.com) based on QSQN & QN Technology commercialized into Mol-Instincts database and ChemRTP, ChemEssen, Inc. (2022).

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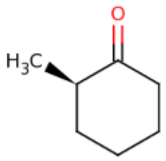
Summary of This Deep Complementary Data Sheet

The table shown below summarizes this Deep Complementary Data Sheet including the target property of the target compound and similar compounds and the availability of the various data. They are helpful to investigate a reliable value and/or range of the target property by analyzing the related data points and/or trends of the data.

Target Property: Normal Boiling Point

Compound	Common Name	QSQN	QN	Existing Approach	Experimental Data	Refined Experimental Data
Target	(2R)-2-Methylcyclohexan-1-one	Available	Available	Available	Available	Available
Similar #1	Cyclohexanone	Available	Available	Available	Available	Available
Similar #2	Cyclohexanol	Available	Available	Available	Available	Available
Similar #3	4-methylcyclohexan-1-one	Available	Available	Available	Available	Available
Similar #4	2,2-dimethylcyclohexan-1-one	Available	Available	Available	Available	Available

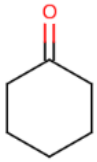
I. Target Compound & Property Data

Common Name of Target Compound: (2R)-2-Methylcyclohexan-1-one	
	CAS Number: 583-60-8 InChI: InChI=1S/C7H12O/c1-6-4-2-3-5-7(6)8/h6H,2-5H2,1H3/t6-/m1/s1 InChIKey: InChIKey=LFSAPCRASZRSKS-ZCFIWIBFSA-N Formula: C7H12O Molecular Weight: 112.1696 g/mol

Property: Normal Boiling Point (K)

Methodology/Source	Value (K)	Reference/Note
QSQN Technology	**435.02**	Click to View the Technology Description...
QN Technology	**435.38**	Click to View the Technology Description...
Joback's Group Contribution Method	**447.13**	Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
Gani's Group Contribution Method	**446.98**	Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *AIChE Journal*, 40(10), 1697-1710.
Experimental Data A total of 22 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.		
Experimental Data 1	**438.15**	Jedlinski, Misioiek, Giowkowski, Janeczek, Wolinska, Tetrahedron; vol. 46; 10; (1990); p. 3547 - 3558
Experimental Data 2	**443.15**	Kessar, Mahajan, Journal of the Indian Chemical Society; vol. 39, (1962) p. 147
Experimental Data 3	**444.15**	Heravi, Majid M. Oskooie, Hossein A. Yazdanpanah, Sedigheh, Mojtahedi, Majid, Journal of Chemical Research 2 (2004) p. 129 - 130
Refined Experimental Data	**438.15**	Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

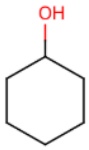
II. Similar Compound #1 & Property Data

Common Name of Similar Compound #1: Cyclohexanone	
	CAS Number: 108-94-1 InChI: InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-5H2 InChIKey: InChIKey=JHIVVAPYMSGYDF-UHFFFAOYSA-N Formula: C6H10O Molecular Weight: 98.1430 g/mol

Property: Normal Boiling Point (K)

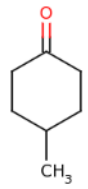
Methodology/Source	Value (K)	Reference/Note
QSQN Technology	**423.20**	Click to View the Technology Description…
QN Technology	**430.61**	Click to View the Technology Description…
Joback's Group Contribution Method	**428.92**	Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
Gani's Group Contribution Method	**433.47**	Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *AIChE Journal*, 40(10), 1697-1710.
Experimental Data A total of 75 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.		
Experimental Data 1	**428.76**	Thermodynamic Data for Pure Compounds. Part A. Hydrocarbons and Ketones, Smith, B.D., Srivastava, R.,1986
Experimental Data 2	**428.75**	J. Appl. Chem. USSR, Marchenko, I.M., Oleneva, O.V., Polyakova, L.V., Mis'ko, I.G., Garber, Yu.N., 1989
Experimental Data 3	**428.58**	J. Chem. Thermo.,Ambrose, D., Ghiassee, N.B., 1987
Refined Experimental Data	**428.58**	Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

III. Similar Compound #2 & Property Data

Common Name of Similar Compound #2: Cyclohexanol	
	CAS Number: 108-93-0 InChI: InChI=1S/C6H12O/c7-6-4-2-1-3-5-6/h6-7H,1-5H2 InChIKey: InChIKey=HPXRVTGHNJAIIH-UHFFFAOYSA-N Formula: C6H12O Molecular Weight: 100.1589 g/mol

Property: Normal Boiling Point (K)		
Methodology/Source	**Value (K)**	**Reference/Note**
QSQN Technology	**440.15**	Click to View the Technology Description…
QN Technology	**436.77**	Click to View the Technology Description…
Joback's Group Contribution Method	**448.61**	Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
Gani's Group Contribution Method	**438.72**	Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *AIChE Journal*, 40(10), 1697-1710.
Experimental Data A total of 49 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.		
Experimental Data 1	**434.25**	Riddick, J.A., Bunger, W.B. Organic Solvents: Physical Properties and Methods of Purification, 3rd ed.(1970)
Experimental Data 2	**434.55**	Timmermans, J. Physico-Chemical Constants of Pure Organic Substances, 2nd ed.(1965)
Experimental Data 3	**434.00**	Stull, D.R., Westrum, E.F.Jr., Sinke, G.C., The Chemical Thermodynamics of Organic Compounds(1969)
Refined Experimental Data	**433.93**	Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

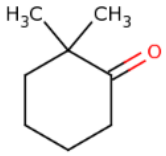
IV. Similar Compound #3 & Property Data

Common Name of Similar Compound #3: **4-methylcyclohexan-1-one**	
	CAS Number: 589-92-4 InChI: InChI=1S/C7H12O/c1-6-2-4-7(8)5-3-6/h6H,2-5H2,1H3 InChIKey: InChIKey=VGVHNLRUAMRIEW-UHFFFAOYSA-N Formula: C7H12O Molecular Weight: 112.1696 g/mol

Property: Normal Boiling Point (K)

Methodology/Source	Value (K)	Reference/Note
QSQN Technology	**443.12**	Click to View the Technology Description...
QN Technology	**441.16**	Click to View the Technology Description...
Joback's Group Contribution Method	**447.13**	Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
Gani's Group Contribution Method	**446.98**	Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *AIChE Journal*, 40(10), 1697-1710.
Experimental Data A total of 13 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.		
Experimental Data 1	**444.65**	Svoboda, Hetflejs, Collection of Czechoslovak Chemical Communications, vol. 42 (1977), p. 2177,2178,2179
Experimental Data 2	**442.65**	Kwart,H. Conley,R.A. Journal of Organic Chemistry, vol. 38 (1973), p. 2011 - 2016
Experimental Data 3	**444.15**	Cetina, Mateos, Journal of Organic Chemistry, vol. 25 (1960), p. 704,706
Refined Experimental Data	**442.02**	Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

V. Similar Compound #4 & Property Data

Common Name of Similar Compound #4: **2,2-dimethylcyclohexan-1-one**	
	CAS Number: 1193-47-1 InChI: InChI=1S/C8H14O/c1-8(2)6-4-3-5-7(8)9/h3-6H2,1-2H3 InChIKey: InChIKey=KNSPBSQWRKKAPI-UHFFFAOYSA-N Formula: C8H14O Molecular Weight: 126.1962 g/mol

Property: Normal Boiling Point (K)

Methodology/Source	Value (K)	Reference/Note
QSQN Technology	**453.59**	Click to View the Technology Description...
QN Technology	**442.85**	Click to View the Technology Description...
Joback's Group Contribution Method	**470.25**	Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
Gani's Group Contribution Method	**459.74**	Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *AIChE Journal*, 40(10), 1697-1710.
Experimental Data A total of 12 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.		
Experimental Data 1	**444.15**	Meyer,W.L. et al. Tetrahedron, vol. 24, (1968), p. 5959 - 5969
Experimental Data 2	**442.65**	Kwart,H. Conley,R.A. Journal of Organic Chemistry, vol. 38 (1973), p. 2011 - 2016
Experimental Data 3	**444.15**	Balsamo et al., Tetrahedron, vol. 29, (1973), p. 199,200,202
Refined Experimental Data	**443.34**	Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

VI. Data Plots

Experimental Data Plot. The experimental data of the target chemical compound and the 4 similar compounds given in the section from **0** to **V** above have been plotted in Figure 1. The number of the data points of each compound is also given in Figure 1. Refined experimental data has been determined as described in the Data Refinement Details.

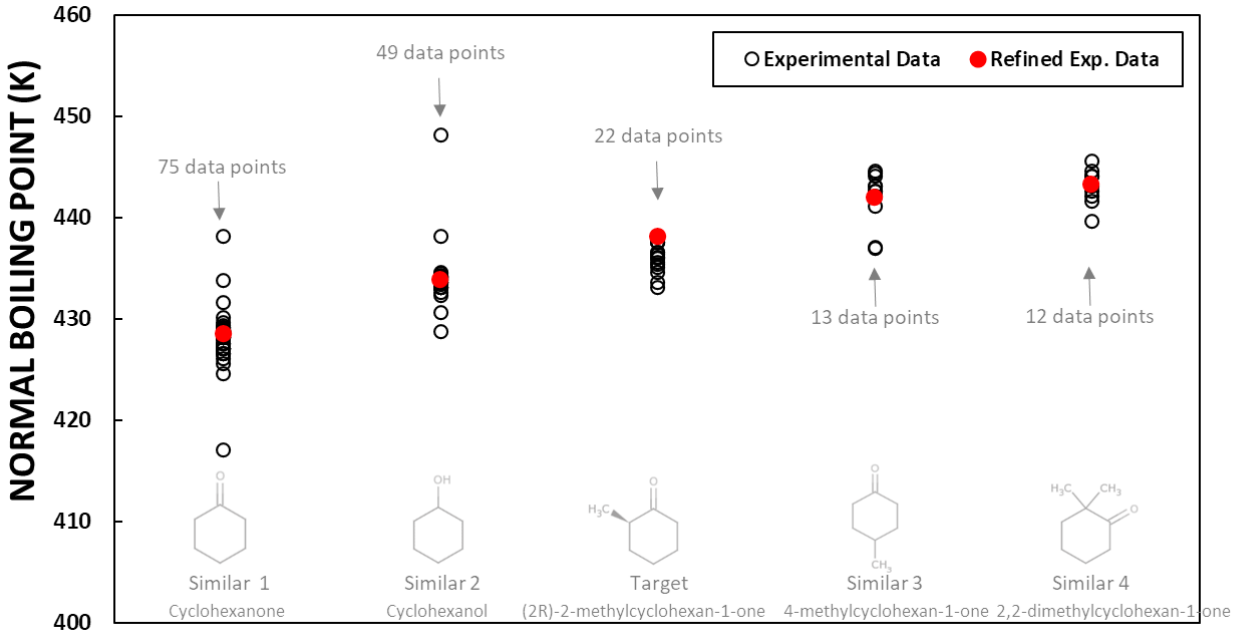


Figure 1. Experimental boiling points of target compound and 4 similar compounds

Computational Data Plot. The plot of the normal boiling points determined by the 4 different approaches is given in Figure 2 together with the refined experimental data and the ranges of the experimental data of each compound.

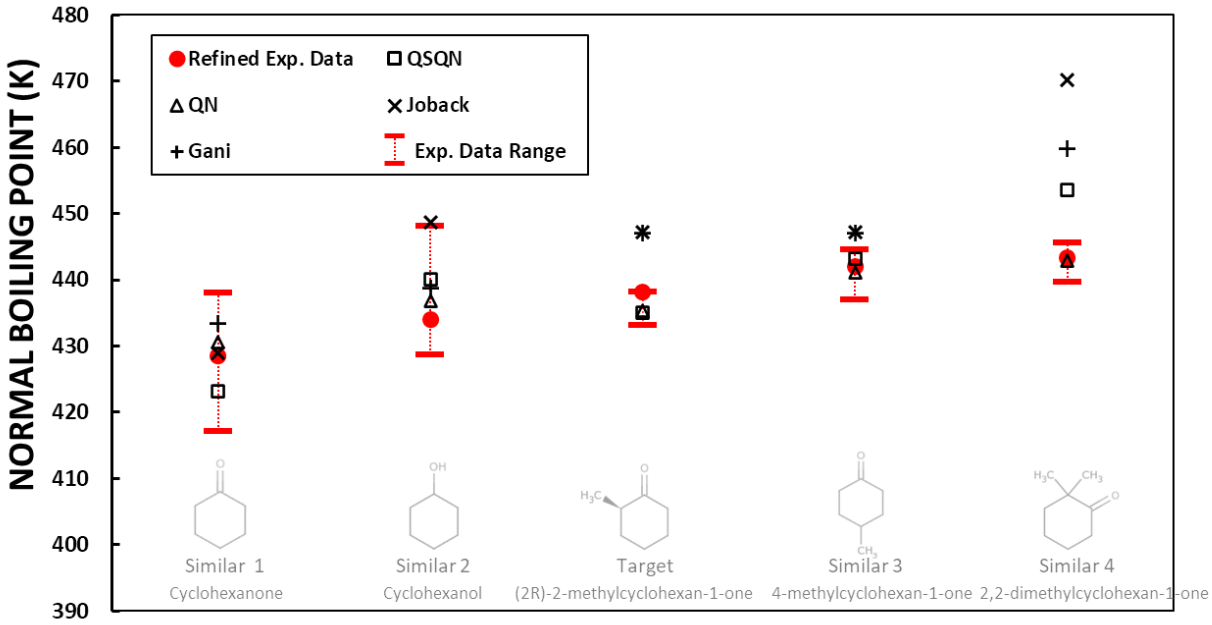


Figure 2. Computational normal boiling points of target and 4 similar compounds

VII. Further Assistance and Services

Contact CCDDS staff at DeepData@Mol-Instincts.com in case you need any further assistance. Refer to the CCDDS homepage for requesting any additional Deep Data or Deep Services.