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

Deep Complementary Data Sheet

(A Sample DCDS: Temperature-Dependent Property Example)

Viscosity of Gas of Methyl Acetate

DCDS-PT10-CT1001349323-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

Viscosity of gas of Methyl Acetate, Deep Complementary Data Sheet (DCDS), No. DCDS-PT10-CT1001349323-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

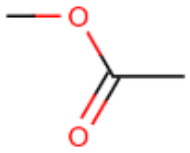
The table shown below summarizes this Deep Complementary Data Sheet including the target property of the target compound and similar compounds and the availability of the various data. They are helpful to investigate a reliable value and/or range of the target property by analyzing the related data points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

Target Property: Viscosity of Gas

Compound	Common Name	QSQN	QN	Existing Approach	Experimental Data	Refined Experimental Data
Target	Methyl Acetate	Available	Available	Available	Available	Available
Similar #1	Ethyl Acetate	Available	Available	Available	Available	Available
Similar #2	Pentyl Acetate	Available	Available	Available	Available	Available
Similar #3	Heptyl Acetate	Available	Available	Available	Available	Available

I. Target Compound & Property Data

Common Name of Target Compound: Methyl Acetate



CAS Number:	79-20-9
InChI:	InChI=1S/C3H6O2/c1-3(4)5-2/h1-2H3
InChIKey:	InChIKey=KXKVLQRXCPHEJC-UHFFFAOYSA-N
Formula:	C3H6O2
Molecular Weight:	74.0785 g/mol

Property: Viscosity of Gas (cP)

Computational Data

Temperature (K)	QSQN Technology (cP)*	Reichenberg (cP)**
178.11	0.004349948	0.005440789
239.83	0.006220039	0.007202423
301.55	0.008061399	0.008903923
363.27	0.009867551	0.010547341
424.98	0.011632014	0.012134659
486.70	0.013348313	0.013667793
548.42	0.015009967	0.015148593
610.14	0.016610499	0.016578844
671.86	0.018143431	0.017960272
733.58	0.019602284	0.019294545

*Click to View the Technology Description...
**Existing Approach: Reichenberg, D., AIChE J., 19: 854 (1973); AIChE J., 21: 181 (1975)

Experimental Data

A total of 12 experimental data points has been collected from the existing publications, which are presented below.

Temperature (K)	Experimental Data (cP)	Reference
293.15	0.00840	K. M. Khalilov, Russ. J. Phys. Chem. 36, 1341 (1962).
503.15	0.01330	
373.15	0.01015	K. Rappenecker, Z. Phys. Chem. Stochiom. Verwandtschaftsl. 72, 695 (1910).
485.65	0.01359	
293.15	0.0084	A. Scholz and G. Kley, Collection of Transport Property Data, TRP-8, 1981.
579.75	0.01583	
416.45	0.01139	Titani, T., Bull. Chem. Soc. Japan (1933).
450.85	0.01236	
491.65	0.01348	
521.35	0.01429	
551.05	0.01508	
579.75	0.01583	

Refined Experimental Data

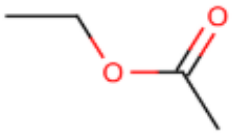
Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

Temperature (K)	Refined Experimental Data (cP)
178.11	0.004349948
239.83	0.006220039

301.55	0.008061399
363.27	0.009867551
424.98	0.011632014
486.70	0.013348313
548.42	0.015009967
610.14	0.016610499
671.86	0.018143431
733.58	0.019602284

II. Similar Compound #1 & Property Data

Common Name of Similar Compound #1: Ethyl Acetate



CAS Number:	141-78-6
InChI:	InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3
InChIKey:	InChIKey=XEKOWRVHYACXOJ-UHFFFAOYSA-N
Formula:	C4H8O2
Molecular Weight:	88.1051 g/mol

Property: Viscosity of Gas (cP)

Computational Data

Temperature (K)	QSQN Technology (cP)*	Reichenberg (cP)**
171.75	0.004780171	0.004204511
237.96	0.006506858	0.005835872
304.17	0.008172445	0.007457497
370.38	0.009779093	0.009059312
436.59	0.011328889	0.010632272
502.80	0.012823845	0.012168922
569.01	0.01426590	0.013663715
635.22	0.015656927	0.015113084
701.43	0.016998732	0.016515288
767.64	0.018293056	0.017870130

*Click to View the Technology Description...

**Existing Approach: Reichenberg, D., AIChE J., 19: 854 (1973); AIChE J., 21: 181 (1975)

Experimental Data

A total of 42 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.

Temperature (K)	Experimental Data (cP)	Reference
373.15	0.009546	Rappenecker, Z. physik. Chem., 72 (1910), 695
485.65	0.0128	
273.10	0.0069	Vogel, H. Ann. Physik (4) 43, 1235-72(1914)
523.00	0.01384	A. G. Nasini, Royal Society, ((1929)
401.25	0.01018	Pal, A.K., Indian J. Phys.(1933)
431.75	0.01098	Reichenberg, D., DSC Rep. 11 (1933)
586.85	0.01497	
466.05	0.01195	Titani, T, Bull. Chem. Soc. Japan (1933)
491.45	0.0125	
521.75	0.01332	
553.25	0.01409	
586.85	0.01497	
333.15	0.0085	K. M. Khalilov, Russ. J. Phys. Chem. 36, 1341 (1962)
493.15	0.0145	
303.65	0.006812	Pal, A. K., Indian J. Phys.(1967)
327.65	0.007529	
473.25	0.01095	
372.35	0.008656	Reichenberg, D. DSC Rep. 11 (1967)
423.35	0.009878	Titani, T., Bull. Chem. Soc. Japan(1967)
473.25	0.01095	

351.60	0.00881	Pal, A.K. Indian J. Phys.(1971)
432.60	0.0108	
189.60	0.00476	Reichenberg, D., National Physical Laboratory, Teddington, England (1971)
270.60	0.0068	
513.60	0.0127	
675.60	0.0164	
756.60	0.0181	
837.60	0.0197	
918.60	0.0213	
999.60	0.0228	
594.60	0.0146	Titani, T., Bull. Chem. Soc. Japan(1971).

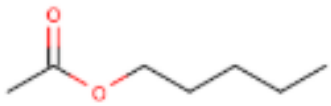
Refined Experimental Data

Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

Temperature (K)	Refined Experimental Data (cP)
171.75	0.004080
237.96	0.005963
304.17	0.007768
370.38	0.009497
436.59	0.011153
502.80	0.012739
569.01	0.014259
635.22	0.015714
701.43	0.017109
767.64	0.018447

III. Similar Compound #2 & Property Data

Common Name of Similar Compound #2: Pentyl Acetate



CAS Number:	141-78-6
InChI:	InChI=1S/C7H14O2/c1-3-4-5-6-9-7(2)8/h3-6H2,1-2H3
InChIKey:	InChIKey=PGMYKACGEOXYJE-UHFFFAOYSA-N
Formula:	C7H14O2
Molecular Weight:	130.1849 g/mol

Property: Viscosity of Gas (cP)

Computational Data

Temperature (K)	QSQN Technology (cP)*	Reichenberg (cP)**
206.44	0.004603577	0.004164151
283.13	0.006201706	0.005719982
359.83	0.007742421	0.007264827
436.53	0.009227782	0.008788896
513.23	0.01065978	0.010283535
589.92	0.012040331	0.011741755
666.62	0.013371283	0.013158509
743.32	0.014654419	0.014530708
820.02	0.015891456	0.015857033
896.71	0.017084051	0.017137623

*Click to View the Technology Description...
**Existing Approach: Reichenberg, D., AIChE J., 19: 854 (1973); AIChE J., 21: 181 (1975)

Experimental Data

A total of 19 experimental points has been collected from the existing publications. Representative points have been selected and presented below.

Temperature (K)	Value (cP)	Reference
425.00	0.00825	Guseinov, K.D., Klimova, T.F., Study on dynamic viscosity of carboxylic-acid esters, Russ. J. Phys. Chem. (1983)
450.00	0.00902	
475.00	0.00979	
500.00	0.01034	
422.15	0.00851	Reichenberg D., "DSC Report 11", National Physical Laboratory, Teddington, England. (1971)
479.15	0.00962	
536.15	0.0107	
593.15	0.0118	
650.15	0.0129	
707.15	0.0139	
764.15	0.0149	
821.15	0.0159	
878.15	0.0168	
935.15	0.0178	
992.15	0.0187	

Refined Experimental Data

Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

Temperature (K)	Refined Experimental Data (cP)

206.44	0.0027974
283.13	0.0049985
359.83	0.0069716
436.53	0.0087489
513.23	0.0103627
589.92	0.0118451
666.62	0.0132285
743.32	0.0145451
820.02	0.0158270
896.71	0.0171065

IV. Similar Compound #3 & Property Data

Common Name of Similar Compound #3: Heptyl Acetate

CAS Number:	112-06-1
InChI:	InChI=1S/C9H18O2/c1-3-4-5-6-7-8-11-9(2)10/h3-8H2,1-2H3
InChIKey:	InChIKey=ZCZSIDMEHXZRLG-UHFFFAOYSA-N
Formula:	C9H18O2
Molecular Weight:	158.2380 g/mol

Property: Viscosity of Gas (cP)

Computational Data

Temperature (K)	QSQN Technology (cP)*	Reichenberg (cP)**
222.95	0.004485101	0.00404579
305.46	0.00603585	0.005551455
387.97	0.007530936	0.007046429
470.49	0.008972356	0.008521257
553.00	0.010362035	0.009967588
635.51	0.011701833	0.011378678
718.02	0.012993538	0.012749659
800.53	0.014238878	0.014077553
883.04	0.015439516	0.01536109
965.56	0.016597057	0.016600405

*Click to View the Technology Description...
**Existing Approach: Reichenberg, D., AIChE J., 19: 854 (1973); AIChE J., 21: 181 (1975)

Experimental Data

A total of 17 experimental data points has been collected from the existing publications. Representative data have been selected and presented below.

Temperature (K)	Experimental Data (cP)	Reference
450.00	0.00852	Reichenberg D., "DSC Report 11", National Physical Laboratory, Teddington, England. (1971)
475.00	0.00912	
500.00	0.00975	
222.95	0.004248	Guseinov, K.D., Klimova, T.F., Study on dynamic viscosity of carboxylic-acid esters, Russ. J. Phys. Chem. (1983)
309.29	0.005902	
395.63	0.007543	
481.97	0.009158	
568.31	0.010739	
654.64	0.012278	
740.98	0.013768	
827.32	0.015207	
913.66	0.016595	
1000.00	0.017932	

Refined Experimental Data

Determined by basic analysis, statistical filtering, and similarity analysis when multiple experimental data exist. Refer to the Data Refinement Details for more information.

Temperature (K)	Refined Experimental Data (cP)
222.95	0.0042225

305.46	0.0058534
387.97	0.0074438
470.49	0.0089933
553.00	0.0105013
635.51	0.0119674
718.02	0.0133909
800.53	0.0147714
883.04	0.0161083
965.56	0.0174011

V. Data Plots

Experimental Data Plot. **The experimental data of the target chemical compound and the 3 similar compounds given in the section from I to IV above have been plotted in** Figure 1 with the trend curves derived from the experimental data and the refined experimental data.

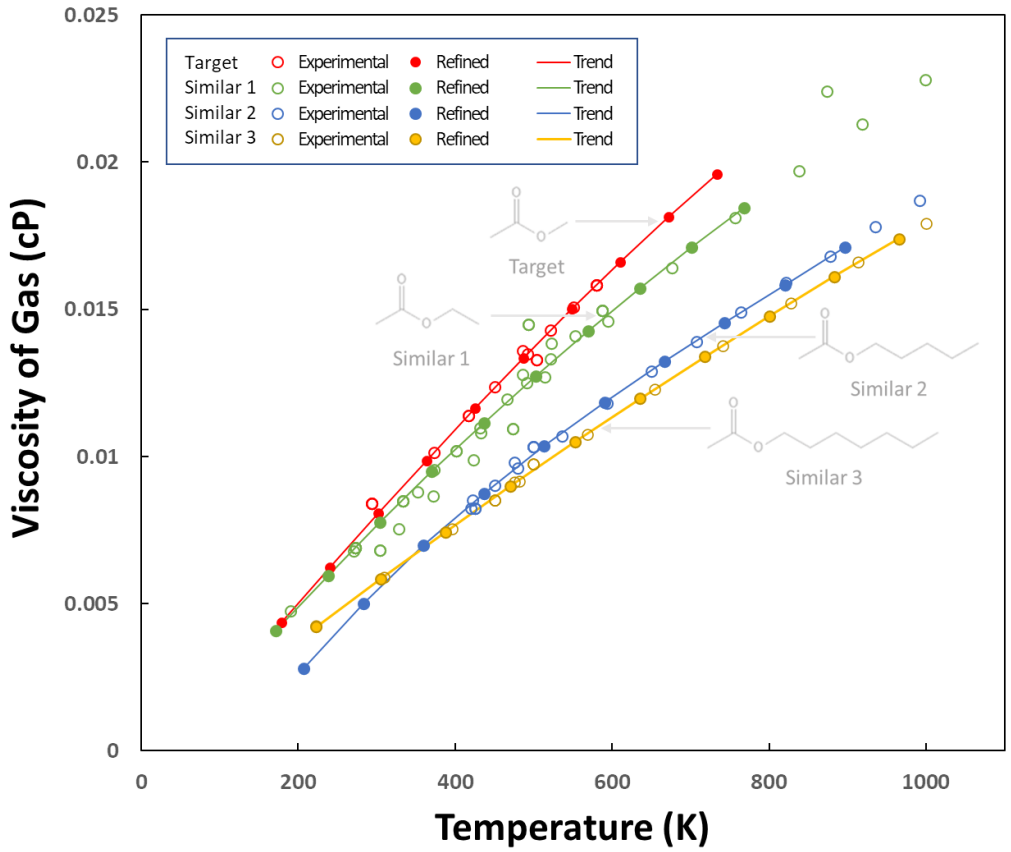


Figure 1. Experimental viscosity of gas of target compound and 3 similar compounds

Computational Data Plot. The plot of the viscosity of gas determined by the 2 different approaches is given in

Figure 2 with the refined experimental data of each compound.

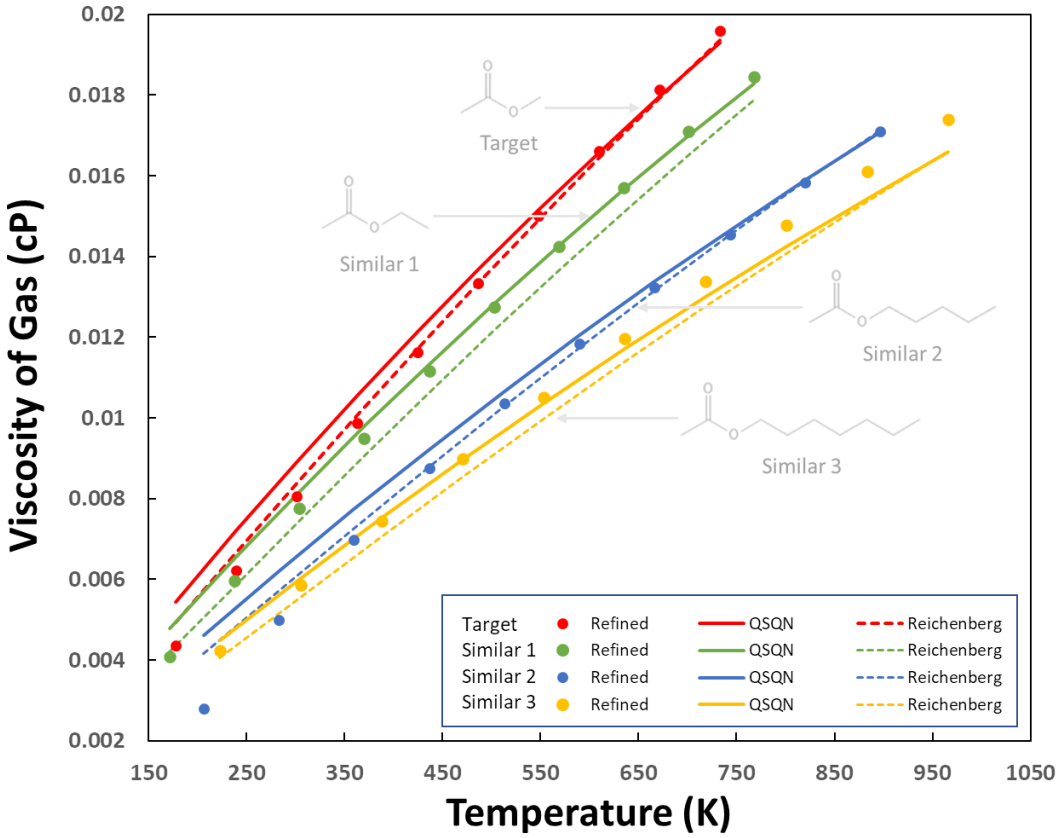


Figure 2. Computational viscosity of gas of target compound and 3 similar compounds

VI. Further 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.