

Cyclohexene, 1,2-dimethyl-

Other names:	1,2-Dimethyl-1-cyclohexene 1,2-Dimethylcyclohexene
Inchi:	InChI=1S/C8H14/c1-7-5-3-4-6-8(7)2/h3-6H2,1-2H3
InchiKey:	TXNWMICHNKMOBR-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1=C(C)CCCC1
Mol. weight [g/mol]:	110.20
CAS:	1674-10-8

Physical Properties

Property code	Value	Unit	Source
gf	59.34	kJ/mol	Joback Method
hf	-98.95	kJ/mol	Joback Method
hfus	7.68	kJ/mol	Joback Method
hvap	35.76	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
tb	388.00 ± 5.00	K	NIST Webbook
tb	408.90 ± 2.00	K	NIST Webbook
tb	439.00 ± 2.00	K	NIST Webbook
tc	622.39	K	Joback Method
tf	189.00 ± 0.01	K	NIST Webbook
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.22	J/mol×K	415.78	Joback Method
cpg	218.13	J/mol×K	450.21	Joback Method
cpg	232.34	J/mol×K	484.65	Joback Method

cpg	245.85	J/mol×K	519.08	Joback Method
cpg	258.70	J/mol×K	553.52	Joback Method
cpg	270.90	J/mol×K	587.95	Joback Method
cpg	282.46	J/mol×K	622.39	Joback Method
dvisc	0.0036526	Pa×s	217.34	Joback Method
dvisc	0.0017220	Pa×s	250.41	Joback Method
dvisc	0.0009675	Pa×s	283.49	Joback Method
dvisc	0.0006132	Pa×s	316.56	Joback Method
dvisc	0.0004237	Pa×s	349.63	Joback Method
dvisc	0.0003120	Pa×s	382.71	Joback Method
dvisc	0.0002413	Pa×s	415.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39946e+01
Coeff. B	-3.26794e+03
Coeff. C	-6.03660e+01
Temperature range (K), min.	298.78
Temperature range (K), max.	436.72

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1674108&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol639.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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