Cyclohexane, 1,2-dimethyl- (cis/trans)

Other names:	1,2-Dimethylcyclohexane
	1,2-dimethylcyclohexane (cis+trans)
	Cyclohexane, 1,2-dimethyl-
	UN 2263
	hexahydro-o-xylene
	o-Dimethylcyclohexane
Inchi:	InChI=1S/C8H16/c1-7-5-3-4-6-8(7)2/h7-8H,3-6H2,1-2H3
InchiKey:	KVZJLSYJROEPSQ-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC1CCCCC1C
Mol. weight [g/mol]:	112.21
CAS:	583-57-3

Physical Properties

Property code	Value	Unit	Source
gf	33.22	kJ/mol	Joback Method
hf	-174.47	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	33.52	kJ/mol	Joback Method
ie	9.45 ± 0.05	eV	NIST Webbook
log10ws	-4.28		Aqueous Solubility Prediction Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	798.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	793.00		NIST Webbook

tb	397.32	K	Joback Method
tc	597.67	K	Joback Method
tf	223.25	K	Aqueous Solubility Prediction Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.47	J/mol×K	597.67	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	247.23	J/mol×K	464.10	Joback Method
cpg	230.28	J/mol×K	430.71	Joback Method
cpg	212.54	J/mol×K	397.32	Joback Method
cpl	173.90	J/mol×K	325.20	NIST Webbook
dvisc	0.0003324	Pa×s	361.61	Joback Method
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method
dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0002631	Pa×s	397.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42946e+01
Coeff. B	-3.35684e+03
Coeff. C	-5.20860e+01
Temperature range (K), min.	291.74
Temperature range (K), max.	425.77

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Miscibility behavior of trihexyl(tetradecyl)phosphonium tetrafluoroborate with cyclic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2014.03.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583573&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
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