1,4-Dimethylcyclohexane

Inchi: InChI=1S/C8H16/c1-7-3-5-8(2)6-4-7/h7-8H,3-6H2,1-2H3
InchiKey: QRMPKOFEUHIBNM-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC1CCC(C)CC1
Mol. weight [g/mol]: 112.21
CAS: 589-90-2

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
log10ws	-4.47		Aqueous Solubility Prediction Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	397.32	K	Joback Method
tc	597.67	K	Joback Method
tf	202.72	K	Aqueous Solubility Prediction Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.54	J/mol×K	397.32	Joback Method
cpg	230.28	J/mol×K	430.71	Joback Method
cpg	247.23	J/mol×K	464.10	Joback Method
cpg	263.41	J/mol×K	497.49	Joback Method
cpg	278.84	J/mol×K	530.89	Joback Method
cpg	293.52	J/mol×K	564.28	Joback Method
cpg	307.47	J/mol×K	597.67	Joback Method

dvisc	0.0041986	Pa×s	183.06	Joback Method
dvisc	0.0018154	Pa×s	218.77	Joback Method
dvisc	0.0009932	Pa×s	254.48	Joback Method
dvisc	0.0006303	Pa×s	290.19	Joback Method
dvisc	0.0004419	Pa×s	325.90	Joback Method
dvisc	0.0003324	Pa×s	361.61	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	1.44557e+01
Coeff. B	-3.37214e+03
Coeff. C	-5.12100e+01
Temperature range (K), min.	289.22
Temperature range (K), max.	419.98

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007236&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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume