

Methylcyclohexane-d14

Inchi:	InChI=1S/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3/i1D3,2D2,3D2,4D2,5D2,6D2,7D
InchiKey:	UAEPNZWRGJTJPN-OBYKGMMLSA-N
Formula:	C7D14
SMILES:	CC1CCCCC1
Mol. weight [g/mol]:	112.27

Physical Properties

Property code	Value	Unit	Source
gf	32.51	kJ/mol	Joback Method
hf	-133.49	kJ/mol	Joback Method
hfus	5.72	kJ/mol	Joback Method
hvap	31.61	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.587		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpola	732.00		NIST Webbook
rinpola	732.00		NIST Webbook
tb	379.11	K	Joback Method
tc	581.63	K	Joback Method
tf	176.03	K	Joback Method
vc	0.360	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.27	J/molxK	379.11	Joback Method
cpg	188.55	J/molxK	412.86	Joback Method
cpg	204.07	J/molxK	446.62	Joback Method
cpg	218.84	J/molxK	480.37	Joback Method
cpg	232.88	J/molxK	514.12	Joback Method
cpg	246.21	J/molxK	547.88	Joback Method
cpg	258.85	J/molxK	581.63	Joback Method
dvisc	0.0077565	Paxs	176.03	Joback Method

dvisc	0.0028475	Paxs	209.88	Joback Method
dvisc	0.0013808	Paxs	243.72	Joback Method
dvisc	0.0007988	Paxs	277.57	Joback Method
dvisc	0.0005205	Paxs	311.42	Joback Method
dvisc	0.0003689	Paxs	345.26	Joback Method
dvisc	0.0002780	Paxs	379.11	Joback Method

Sources

Miscibility behavior of trihexyl(tetradecyl)phosphonium hexafluorophosphate with cyclic hydrocarbons: McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2014.03.020>

NIST Webbook:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R136620&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

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
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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