

1,1':3',1''-Tercyclohexane

Other names:	1,3-(Dicyclohexyl)cyclohexane m-Tercyclohexane m-Tercyclohexyl 1,3-Tercyclohexyl
Inchi:	InChI=1S/C18H32/c1-3-8-15(9-4-1)17-12-7-13-18(14-17)16-10-5-2-6-11-16/h15-18H,1-14H
InchiKey:	JBQRJHVXZMSLNH-UHFFFAOYSA-N
Formula:	C18H32
SMILES:	C1CCC(C2CCCC(C3CCCCC3)C2)CC1
Mol. weight [g/mol]:	248.45
CAS:	1706-50-9

Physical Properties

Property code	Value	Unit	Source
chl	-11114.20	kJ/mol	NIST Webbook
gf	166.32	kJ/mol	Joback Method
hf	-272.23	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.953		Crippen Method
mcvol	231.900	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
tb	665.22	K	Joback Method
tc	910.58	K	Joback Method
tf	310.52	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.61	J/mol×K	910.58	Joback Method
cpg	715.88	J/mol×K	665.22	Joback Method
cpg	851.05	J/mol×K	869.69	Joback Method
cpg	828.44	J/mol×K	828.79	Joback Method

cpg	803.71	J/mol×K	787.90	Joback Method
cpg	776.76	J/mol×K	747.01	Joback Method
cpg	747.51	J/mol×K	706.11	Joback Method
cpl	457.30	J/mol×K	311.00	NIST Webbook
cpl	502.10	J/mol×K	373.00	NIST Webbook
dvisc	0.0002388	Pa×s	606.10	Joback Method
dvisc	0.0003492	Pa×s	546.99	Joback Method
dvisc	0.0005598	Pa×s	487.87	Joback Method
dvisc	0.0010222	Pa×s	428.75	Joback Method
dvisc	0.0022628	Pa×s	369.64	Joback Method
dvisc	0.0067794	Pa×s	310.52	Joback Method
dvisc	0.0001748	Pa×s	665.22	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1706509&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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