1,1':2',1''-Tercyclohexane

Other names:	1,1':2',1''-Tercyclohexyl
	1,2-Dicyclohexylcyclohexane
	1,2-Tercyclohexyl
	o-Tercyclohexyl
Inchi:	InChI=1S/C18H32/c1-3-9-15(10-4-1)17-13-7-8-14-18(17)16-11-5-2-6-12-16/h15-18H,1-14
InchiKey:	JSVILEFZXZLOES-UHFFFAOYSA-N
Formula:	C18H32
SMILES:	C1CCC(C2CCCCC2C2CCCCC2)CC1
Mol. weight [g/mol]:	248.45
CAS:	2456-43-1

Physical Properties

Property code	Value	Unit	Source
chl	-11147.20	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	270.00 ± 0.33	K	NIST Webbook
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.05	J/mol×K	869.69	Joback Method
cpg	715.88	J/mol×K	665.22	Joback Method
cpg	747.51	J/mol×K	706.11	Joback Method
cpg	776.76	J/mol×K	747.01	Joback Method

cpg	803.71	J/mol×K	787.90	Joback Method
cpg	828.44	J/mol×K	828.79	Joback Method
cpg	871.61	J/mol×K	910.58	Joback Method
cpl	424.30	J/mol×K	311.00	NIST Webbook
cpl	427.20	J/mol×K	313.00	NIST Webbook
dvisc	0.0001748	Pa×s	665.22	Joback Method
dvisc	0.0067794	Pa×s	310.52	Joback Method
dvisc	0.0022628	Pa×s	369.64	Joback Method
dvisc	0.0010222	Pa×s	428.75	Joback Method
dvisc	0.0005598	Pa×s	487.87	Joback Method
dvisc	0.0003492	Pa×s	546.99	Joback Method
dvisc	0.0002388	Pa×s	606.10	Joback Method
hvapt	72.80	kJ/mol	469.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68954e+01
Coeff. B	-6.90627e+03
Coeff. C	-3.71390e+01
Temperature range (K), min.	453.15
Temperature range (K), max.	633.15

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2456431&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
hvapt:	Enthalpy of vaporization at a given temperature
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