1,1,10,10-Tetramethylcyclooctadecane

Inchi: InChI=1S/C22H44/c1-21(2)17-13-9-5-7-11-15-19-22(3,4)20-16-12-8-6-10-14-18-21/h5-20
InchiKey: HEYYLLOULCSVBY-UHFFFAOYSA-N
Formula: C22H44
SMILES: CC1(C)CCCCCCCCC(C)(C)CCCCCCCC1
Mol. weight [g/mol]: 308.58
CAS: 23014-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-5.08	kJ/mol	Joback Method
hf	-506.87	kJ/mol	Joback Method
hfus	7.85	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.294		Crippen Method
mcvol	309.980	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
tb	769.36	K	Joback Method
tc	1025.27	K	Joback Method
tf	359.00 ± 1.00	K	NIST Webbook
tf	359.00 ± 0.20	K	NIST Webbook
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.08	J/mol×K	769.36	Joback Method
cpg	1045.86	J/mol×K	812.01	Joback Method
cpg	1079.59	J/mol×K	854.66	Joback Method
cpg	1111.49	J/mol×K	897.32	Joback Method
cpg	1141.77	J/mol×K	939.97	Joback Method
cpg	1170.65	J/mol×K	982.62	Joback Method
cpg	1198.35	J/mol×K	1025.27	Joback Method
hfust	39.58	kJ/mol	359.00	NIST Webbook

hfust	39.58	kJ/mol	359.20	NIST Webbook
sfust	110.00	J/mol×K	359.00	NIST Webbook

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=C23014564&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume