Cyclohexene, 1,6,6-trimethyl-

Other names: 2,3,3-Trimethylcyclohexene
Inchi: InChI=1S/C9H16/c1-8-6-4-5-7-9(8,2)3/h6H,4-5,7H2,1-3H3
InchiKey: UBMLKGCOROJNMF-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1=CCCCC1(C)C
Mol. weight [g/mol]: 124.22
CAS: 69745-49-9

Physical Properties

Property code	Value	Unit	Source
gf	64.19	kJ/mol	Joback Method
hf	-113.22	kJ/mol	Joback Method
hfus	5.44	kJ/mol	Joback Method
hvap	35.86	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	420.00 ± 0.30	K	NIST Webbook
tc	640.93	K	Joback Method
tf	200.17 ± 0.30	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.07	J/mol×K	429.25	Joback Method
cpg	261.48	J/mol×K	464.53	Joback Method
cpg	277.72	J/mol×K	499.81	Joback Method
cpg	292.91	J/mol×K	535.09	Joback Method
cpg	307.14	J/mol×K	570.37	Joback Method
cpg	320.51	J/mol×K	605.65	Joback Method
cpg	333.12	J/mol×K	640.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69745499&Units=SI
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

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