3,3-Dimethylcyclohexene

Inchi: InChI=1S/C8H14/c1-8(2)6-4-3-5-7-8/h4,6H,3,5,7H2,1-2H3
InchiKey: BWYHTITWPWGSHN-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC1(C)C=CCCC1
Mol. weight [g/mol]: 110.20
CAS: 695-28-3

Physical Properties

Property code	Value	Unit	Source
gf	65.40	kJ/mol	Joback Method
hf	-81.11	kJ/mol	Joback Method
hfus	3.24	kJ/mol	Joback Method
hvap	32.97	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.753		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	401.39	K	Joback Method
tc	613.90	K	Joback Method
tf	211.96	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.60	J/mol×K	401.39	Joback Method
cpg	217.67	J/mol×K	436.81	Joback Method
cpg	233.51	J/mol×K	472.23	Joback Method
cpg	248.21	J/mol×K	507.65	Joback Method
cpg	261.88	J/mol×K	543.07	Joback Method
cpg	274.63	J/mol×K	578.48	Joback Method
cpg	286.57	J/mol×K	613.90	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol644.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C695283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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