3,3-dimethylcyclopentene

Inchi: InChI=1S/C7H12/c1-7(2)5-3-4-6-7/h3,5H,4,6H2,1-2H3
InchiKey: FONFXXNTLGAHGI-UHFFFAOYSA-N
Formula: C7H12
SMILES: CC1(C)C=CCC1
Mol. weight [g/mol]: 96.17
CAS: 58049-91-5

Physical Properties

Property code	Value	Unit	Source
gf	69.08	kJ/mol	Joback Method
hf	-54.31	kJ/mol	Joback Method
hfus	2.75	kJ/mol	Joback Method
hvap	30.57	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	351.40 ± 2.00	K	NIST Webbook
tb	350.90 ± 2.00	K	NIST Webbook
tc	579.63	K	Joback Method
tf	204.21	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.74	J/mol×K	374.24	Joback Method
cpg	177.82	J/mol×K	408.47	Joback Method
cpg	191.74	J/mol×K	442.70	Joback Method
cpg	204.60	J/mol×K	476.93	Joback Method
cpg	216.48	J/mol×K	511.16	Joback Method
cpg	227.50	J/mol×K	545.39	Joback Method
cpg	237.75	J/mol×K	579.63	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol623.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58049915&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

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