3,3-Dimethyl-6-methylenecyclohexene

Inchi: InChI=1S/C9H14/c1-8-4-6-9(2,3)7-5-8/h4,6H,1,5,7H2,2-3H3
InchiKey: AAHPXHCHLLIBGH-UHFFFAOYSA-N
Formula: C9H14
SMILES: C=C1C=CC(C)(C)CC1
Mol. weight [g/mol]: 122.21
CAS: 20185-16-4

Physical Properties

Property code	Value	Unit	Source
gf	126.90	kJ/mol	Joback Method
hf	-17.51	kJ/mol	Joback Method
hfus	4.67	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	996.80		NIST Webbook
rinpol	996.80		NIST Webbook
rinpol	996.80		NIST Webbook
tb	423.43	K	Joback Method
tc	635.60	K	Joback Method
tf	236.91	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.73	J/mol×K	423.43	Joback Method
cpg	245.03	J/mol×K	458.79	Joback Method
cpg	260.20	J/mol×K	494.15	Joback Method
cpg	274.33	J/mol×K	529.52	Joback Method
cpg	287.53	J/mol×K	564.88	Joback Method
cpg	299.90	J/mol×K	600.24	Joback Method

cpg	311.54	J/mol×K	635.60	Joback Method

Sources

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=C20185164&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume