Cyclohexene, 1,3-diisopropenyl-6-methyl-

Other names: Cyclohexene, 1,3-diisopropenyl-6-me
Inchi: InChI=1S/C13H20/c1-9(2)12-7-6-11(5)13(8-12)10(3)4/h8,11-12H,1,3,6-7H2,2,4-5H3
InchiKey: SFWPBBHYROOSNZ-UHFFFAOYSA-N
Formula: C13H20
SMILES: C=C(C)C1=CC(C(=C)C)CCC1C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	254.23	kJ/mol	Joback Method
hf	-0.08	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.111		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
tb	508.98	K	Joback Method
tc	717.20	K	Joback Method
tf	221.25	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.82	J/mol×K	508.98	Joback Method
cpg	411.01	J/mol×K	543.68	Joback Method
cpg	430.13	J/mol×K	578.39	Joback Method
cpg	448.20	J/mol×K	613.09	Joback Method
cpg	465.27	J/mol×K	647.79	Joback Method
cpg	481.37	J/mol×K	682.49	Joback Method
cpg	496.54	J/mol×K	717.20	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=U151289&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