1,3,5,6-Tetramethyladamantane

Other names: 1,2,5,7-tetramethyladamantane
Inchi: InChI=1S/C14H24/c1-10-11-5-12(2)7-13(3,6-11)9-14(10,4)8-12/h10-11H,5-9H2,1-4H3
InchiKey: HBIKNLNXSSBQCT-UHFFFAOYSA-N
Formula: C14H24
SMILES: CC1C2CC3(C)CC(C)(C2)CC1(C)C3
Mol. weight [g/mol]: 192.34
CAS: 34694-70-7

Physical Properties

Property code	Value	Unit	Source
gf	205.26	kJ/mol	Joback Method
hf	-115.01	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	42.60	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.249		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1225.00		NIST Webbook
tb	535.59	K	Joback Method
tc	763.15	K	Joback Method
tf	361.06	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.93	J/mol×K	535.59	Joback Method
cpg	491.25	J/mol×K	573.52	Joback Method
cpg	512.64	J/mol×K	611.44	Joback Method
cpg	532.52	J/mol×K	649.37	Joback Method
cpg	551.29	J/mol×K	687.29	Joback Method
cpg	569.38	J/mol×K	725.22	Joback Method
cpg	587.20	J/mol×K	763.15	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=C34694707&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