1,3,6-Trimethyladamantane

Inchi: InChI=1S/C13H22/c1-9-10-4-12(2)5-11(9)7-13(3,6-10)8-12/h9-11H,4-8H2,1-3H3
InchiKey: NTCDHPNMXULVMK-UHFFFAOYSA-N
Formula: C13H22
SMILES: CC1C2CC3(C)CC1CC(C)(C2)C3
Mol. weight [g/mol]: 178.31
CAS: 24139-37-5

Physical Properties

Property code	Value	Unit	Source
gf	202.33	kJ/mol	Joback Method
hf	-109.61	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	41.52	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.859		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1189.00		NIST Webbook
tb	512.47	K	Joback Method
tc	734.57	K	Joback Method
tf	325.89	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.67	J/mol×K	512.47	Joback Method
cpg	440.84	J/mol×K	549.49	Joback Method
cpg	462.14	J/mol×K	586.50	Joback Method
cpg	481.85	J/mol×K	623.52	Joback Method
cpg	500.27	J/mol×K	660.54	Joback Method
cpg	517.68	J/mol×K	697.56	Joback Method
cpg	534.37	J/mol×K	734.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24139375&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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