1,4-Dimethyladamantane, # 2

Inchi: InChI=1S/C12H20/c1-8-10-3-9-4-11(8)7-12(2,5-9)6-10/h8-11H,3-7H2,1-2H3
InchiKey: MUQFEEYWQQZABK-UHFFFAOYSA-N
Formula: C12H20
SMILES: CC1C2CC3CC1CC(C)(C3)C2
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	199.40	kJ/mol	Joback Method
hf	-104.21	kJ/mol	Joback Method
hfus	14.99	kJ/mol	Joback Method
hvap	40.45	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.469		Crippen Method
mcvol	147.360	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1211.00		NIST Webbook
tb	489.35	K	Joback Method
tc	705.73	K	Joback Method
tf	290.72	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.92	J/mol×K	489.35	Joback Method
cpg	390.71	J/mol×K	525.41	Joback Method
cpg	411.78	J/mol×K	561.48	Joback Method
cpg	431.34	J/mol×K	597.54	Joback Method
cpg	449.56	J/mol×K	633.60	Joback Method
cpg	466.61	J/mol×K	669.67	Joback Method
cpg	482.69	J/mol×K	705.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142551&Units=SI

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