2,2-dimethyladamantane

Inchi: InChI=1S/C12H20/c1-12(2)10-4-8-3-9(6-10)7-11(12)5-8/h8-11H,3-7H2,1-2H3
InchiKey: KOLCSQBNCFAWAM-UHFFFAOYSA-N
Formula: C12H20
SMILES: CC1(C)C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 164.29
CAS: 19740-34-2

Physical Properties

Property code	Value	Unit	Source
chs	-7324.00 ± 3.00	kJ/mol	NIST Webbook
gf	199.40	kJ/mol	Joback Method
hf	-183.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-256.00 ± 3.00	kJ/mol	NIST Webbook
hfus	14.99	kJ/mol	Joback Method
hsub	73.60 ± 1.30	kJ/mol	NIST Webbook
hsub	73.00	kJ/mol	NIST Webbook
hsub	74.00 ± 1.00	kJ/mol	NIST Webbook
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	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1269.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1500.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19740342&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume