

1e,4a-dimethyladamantane

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/t8?,9-,10-,11-
InchiKey: MUQFEEYWQQZABK-BJWRHGQKSA-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
rinpol	1221.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1216.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1395.00		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=R383841&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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