1-ethyl-3,5,7-trimethyladamantane

Inchi: InChI=1S/C15H26/c1-5-15-9-12(2)6-13(3,10-15)8-14(4,7-12)11-15/h5-11H2,1-4H3/t12-,1
InchiKey: XJPFDAWKYDBNOI-DGKWVBSXSA-N
Formula: C15H26
SMILES: CCC12CC3(C)CC(C)(CC(C)(C3)C1)C2
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	215.90	kJ/mol	Joback Method
hf	-100.07	kJ/mol	Joback Method
hfus	2.79	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.783		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	563.38	K	Joback Method
tc	796.14	K	Joback Method
tf	400.47	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.85	J/mol×K	563.38	Joback Method
cpg	540.55	J/mol×K	602.17	Joback Method
cpg	561.47	J/mol×K	640.97	Joback Method
cpg	581.16	J/mol×K	679.76	Joback Method

cpg	600.20	J/mol×K	718.55	Joback Method
cpg	619.13	J/mol×K	757.34	Joback Method
cpg	638.51	J/mol×K	796.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134491&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