1,3-diethyl-5-methyladamantane

Inchi: InChI=1S/C15H26/c1-4-14-7-12-6-13(3,9-14)10-15(5-2,8-12)11-14/h12H,4-11H2,1-3H3/t
InchiKey: YENQWKFWURXCBW-DGKWVBSXSA-N
Formula: C15H26
SMILES: CCC12CC3CC(C)(C1)CC(CC)(C3)C2
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	221.39	kJ/mol	Joback Method
hf	-115.31	kJ/mol	Joback Method
hfus	9.09	kJ/mol	Joback Method
hvap	45.13	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.783		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
tb	563.14	K	Joback Method
tc	786.58	K	Joback Method
tf	376.57	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.98	J/mol×K	563.14	Joback Method
cpg	541.76	J/mol×K	600.38	Joback Method
cpg	562.86	J/mol×K	637.62	Joback Method
cpg	582.68	J/mol×K	674.86	Joback Method
cpg	601.64	J/mol×K	712.10	Joback Method
cpg	620.12	J/mol×K	749.34	Joback Method
cpg	638.53	J/mol×K	786.58	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=R134486&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