1,3-diethyl-5,7-dimethyladamantane

Inchi: InChI=1S/C16H28/c1-5-15-8-13(3)7-14(4,9-15)11-16(6-2,10-13)12-15/h5-12H2,1-4H3/t13
InchiKey: DEHQKWLNZJQUTD-PJPHBNEVSA-N
Formula: C16H28
SMILES: CCC12CC3(C)CC(C)(C1)CC(CC)(C3)C2
Mol. weight [g/mol]: 220.39

Physical Properties

Property code	Value	Unit	Source
gf	224.32	kJ/mol	Joback Method
hf	-120.71	kJ/mol	Joback Method
hfus	5.38	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.173		Crippen Method
mcvol	203.720	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	586.26	K	Joback Method
tc	814.51	K	Joback Method
tf	411.74	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.97	J/mol×K	586.26	Joback Method
cpg	592.76	J/mol×K	624.30	Joback Method
cpg	614.04	J/mol×K	662.34	Joback Method
cpg	634.36	J/mol×K	700.38	Joback Method
cpg	654.24	J/mol×K	738.42	Joback Method
cpg	674.22	J/mol×K	776.46	Joback Method
cpg	694.82	J/mol×K	814.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134471&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

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