1,3-Diethyladamantane

Inchi: InChI=1S/C14H24/c1-3-13-6-11-5-12(7-13)9-14(4-2,8-11)10-13/h11-12H,3-10H2,1-2H3
InchiKey: XHQDEOWLMBIVBU-UHFFFAOYSA-N
Formula: C14H24
SMILES: CCC12CC3CC(C1)CC(CC)(C3)C2
Mol. weight [g/mol]: 192.34
CAS: 25074-51-5

Physical Properties

Property code	Value	Unit	Source
gf	218.46	kJ/mol	Joback Method
hf	-109.91	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.393		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
tb	540.02	K	Joback Method
tc	758.43	K	Joback Method
tf	341.40	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.15	J/mol×K	540.02	Joback Method
cpg	490.88	J/mol×K	576.42	Joback Method
cpg	511.89	J/mol×K	612.82	Joback Method
cpg	531.47	J/mol×K	649.22	Joback Method

cpg	549.91	J/mol×K	685.63	Joback Method
cpg	567.49	J/mol×K	722.03	Joback Method
cpg	584.51	J/mol×K	758.43	Joback Method

Sources

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=C25074515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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