1,2-Diethyladamantane

Inchi: InChI=1S/C14H24/c1-3-13-12-6-10-5-11(7-12)9-14(13,4-2)8-10/h10-13H,3-9H2,1-2H3
InchiKey: VELCHXSEKJBSKL-UHFFFAOYSA-N
Formula: C14H24
SMILES: CCC1C2CC3CC(C2)CC1(CC)C3
Mol. weight [g/mol]: 192.34

Physical Properties

Property code	Value	Unit	Source
gf	216.24	kJ/mol	Joback Method
hf	-145.49	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	44.90	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.249		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1243.00		NIST Webbook
tb	535.11	K	Joback Method
tc	744.74	K	Joback Method
tf	313.26	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.88	J/mol×K	535.11	Joback Method
cpg	492.11	J/mol×K	570.05	Joback Method
cpg	513.78	J/mol×K	604.99	Joback Method
cpg	534.07	J/mol×K	639.92	Joback Method
cpg	553.15	J/mol×K	674.86	Joback Method
cpg	571.18	J/mol×K	709.80	Joback Method
cpg	588.35	J/mol×K	744.74	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=R142482&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

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