1,3-Dehydroadamantane

Inchi: InChI=1S/C10H14/c1-7-2-9-4-8(1)5-10(9,3-7)6-9/h7-8H,1-6H2
InchiKey: YNLPLYJBYLQXCY-UHFFFAOYSA-N
Formula: C10H14
SMILES: C1C2CC34CC1CC3(C2)C4
Mol. weight [g/mol]: 134.22
CAS: 24569-89-9

Physical Properties

Property code	Value	Unit	Source
gf	289.54	kJ/mol	Joback Method
hf	84.27	kJ/mol	Joback Method
hfus	5.80	kJ/mol	Joback Method
hvap	34.86	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.587		Crippen Method
mcvol	108.320	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	447.10	K	Joback Method
tc	672.39	K	Joback Method
tf	329.06	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.21	J/mol×K	447.10	Joback Method
cpg	281.20	J/mol×K	484.65	Joback Method
cpg	298.73	J/mol×K	522.20	Joback Method
cpg	314.17	J/mol×K	559.75	Joback Method
cpg	327.89	J/mol×K	597.29	Joback Method
cpg	340.26	J/mol×K	634.84	Joback Method
cpg	351.65	J/mol×K	672.39	Joback Method

Sources

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=C24569899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume