2,4-Methano-2,4-didehydroadamantane

Inchi: InChI=1S/C11H14/c1-6-2-8-4-7(1)10-5-11(8,10)9(10)3-6/h6-9H,1-5H2
InchiKey: BYDHYGGDDSJOII-UHFFFAOYSA-N
Formula: C11H14
SMILES: C1C2CC3CC1C14CC31C4C2
Mol. weight [g/mol]: 146.23
CAS: 73586-31-9

Physical Properties

Property code	Value	Unit	Source
gf	375.20	kJ/mol	Joback Method
hf	128.41	kJ/mol	Joback Method
hfus	11.80	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.442		Crippen Method
mcvol	111.550	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	463.51	K	Joback Method
tc	685.71	K	Joback Method
tf	361.07	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.08	J/mol×K	463.51	Joback Method
cpg	313.09	J/mol×K	500.54	Joback Method
cpg	330.60	J/mol×K	537.58	Joback Method
cpg	345.99	J/mol×K	574.61	Joback Method
cpg	359.68	J/mol×K	611.64	Joback Method
cpg	372.05	J/mol×K	648.68	Joback Method
cpg	383.51	J/mol×K	685.71	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=C73586319&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
ie:	Ionization energy
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