[3.3.3]Propellane, 2-methylene-

Inchi: InChI=1S/C12H18/c1-10-4-9-11-5-2-7-12(10,11)8-3-6-11/h1-9H2
InchiKey: JRBVAAGYBLRKMS-UHFFFAOYSA-N
Formula: C12H18
SMILES: C=C1CCC23CCCC12CCC3
Mol. weight [g/mol]: 162.27
CAS: 111917-14-7

Physical Properties

Property code	Value	Unit	Source
gf	258.02	kJ/mol	Joback Method
hf	50.13	kJ/mol	Joback Method
hfus	2.22	kJ/mol	Joback Method
hvap	40.56	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-3.90		Crippen Method
logp	3.677		Crippen Method
mcvol	143.060	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	507.03	K	Joback Method
tc	744.52	K	Joback Method
tf	337.50	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.74	J/mol×K	507.03	Joback Method
cpg	371.70	J/mol×K	546.61	Joback Method
cpg	390.64	J/mol×K	586.19	Joback Method
cpg	407.92	J/mol×K	625.78	Joback Method
cpg	423.91	J/mol×K	665.36	Joback Method
cpg	438.97	J/mol×K	704.94	Joback Method
cpg	453.44	J/mol×K	744.52	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=C111917147&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
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