[1.1.1]Propellane

Inchi: InChI=1S/C5H6/c1-4-2-5(1,4)3-4/h1-3H2
InchiKey: ZTXSPLGEGCABFL-UHFFFAOYSA-N
Formula: C5H6
SMILES: C1C23CC12C3
Mol. weight [g/mol]: 66.10
CAS: 35634-10-7

Physical Properties

Property code	Value	Unit	Source
gf	218.60	kJ/mol	Joback Method
hf	147.33	kJ/mol	Joback Method
hfus	-2.16	kJ/mol	Joback Method
hvap	23.78	kJ/mol	Joback Method
ie	9.74	eV	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.170		Crippen Method
mcvol	48.730	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	322.09	K	Joback Method
tc	519.85	K	Joback Method
tf	266.05	K	Joback Method
vc	0.215	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.78	J/mol×K	322.09	Joback Method
cpg	92.79	J/mol×K	355.05	Joback Method
cpg	105.51	J/mol×K	388.01	Joback Method
cpg	116.18	J/mol×K	420.97	Joback Method
cpg	125.03	J/mol×K	453.93	Joback Method
cpg	132.28	J/mol×K	486.89	Joback Method
cpg	138.19	J/mol×K	519.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35634107&Units=SI
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

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