[3.3.3]Propellane, 2,8-bis(methylene)-

Inchi: InChI=1S/C13H18/c1-10-4-8-12-6-3-7-13(10,12)11(2)5-9-12/h1-9H2
InchiKey: WOEZXEPTVDIMMB-UHFFFAOYSA-N
Formula: C13H18
SMILES: C=C1CCC23CCCC12C(=C)CC3
Mol. weight [g/mol]: 174.28
CAS: 112112-57-9

Physical Properties

Property code	Value	Unit	Source
gf	319.52	kJ/mol	Joback Method
hf	113.73	kJ/mol	Joback Method
hfus	3.65	kJ/mol	Joback Method
hvap	42.94	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-4.17		Crippen Method
logp	3.843		Crippen Method
mcvol	152.850	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	529.07	K	Joback Method
tc	764.26	K	Joback Method
tf	362.45	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.24	J/mol×K	529.07	Joback Method
cpg	399.99	J/mol×K	568.27	Joback Method
cpg	417.99	J/mol×K	607.47	Joback Method
cpg	434.57	J/mol×K	646.66	Joback Method
cpg	450.08	J/mol×K	685.86	Joback Method
cpg	464.86	J/mol×K	725.06	Joback Method
cpg	479.25	J/mol×K	764.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112112579&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