[3.3.3]Propellane-2,8-dione, 9-methylene-

Inchi: InChI=1S/C12H14O2/c1-8-2-5-11-6-3-9(13)12(8,11)10(14)4-7-11/h1-7H2
InchiKey: XOUFDVRLVGVXSP-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: C=C1CCC23CCC(=O)C12C(=O)CC3
Mol. weight [g/mol]: 190.24
CAS: 112112-58-0

Physical Properties

Property code	Value	Unit	Source
gf	12.84	kJ/mol	Joback Method
hf	-225.27	kJ/mol	Joback Method
hfus	1.24	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
ie	8.77	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.035		Crippen Method
mcvol	146.200	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	642.67	K	Joback Method
tc	909.29	K	Joback Method
tf	473.94	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.99	J/mol×K	642.67	Joback Method
cpg	430.94	J/mol×K	687.11	Joback Method
cpg	448.04	J/mol×K	731.54	Joback Method
cpg	464.68	J/mol×K	775.98	Joback Method
cpg	481.26	J/mol×K	820.42	Joback Method
cpg	498.16	J/mol×K	864.85	Joback Method
cpg	515.76	J/mol×K	909.29	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=C112112580&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