[3.3.3]Propellane-2,8-dione

Inchi: InChI=1S/C11H14O2/c12-8-2-6-10-4-1-5-11(8,10)9(13)3-7-10/h1-7H2
InchiKey: AJSCTGYMIJHROB-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: O=C1CCC23CCCC12C(=O)CC3
Mol. weight [g/mol]: 178.23
CAS: 112138-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-48.66	kJ/mol	Joback Method
hf	-288.87	kJ/mol	Joback Method
hfus	-0.20	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.869		Crippen Method
mcvol	136.410	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	620.63	K	Joback Method
tc	891.47	K	Joback Method
tf	448.99	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.71	J/mol×K	620.63	Joback Method
cpg	404.28	J/mol×K	665.77	Joback Method
cpg	421.77	J/mol×K	710.91	Joback Method
cpg	438.59	J/mol×K	756.05	Joback Method
cpg	455.17	J/mol×K	801.19	Joback Method
cpg	471.92	J/mol×K	846.33	Joback Method
cpg	489.26	J/mol×K	891.47	Joback Method

Sources

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=C112138348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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