4,8-Dimethylbicyclo[3.3.1]nonane-2,6-dione

Other names: 4,8-Dimethylbicyclo[3.3.1]nona-2,6-dione
Inchi: InChI=1S/C11H16O2/c1-6-3-10(12)9-5-8(6)11(13)4-7(9)2/h6-9H,3-5H2,1-2H3
InchiKey: OTBXXMWIANCGFF-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC1CC(=O)C2CC1C(=O)CC2C
Mol. weight [g/mol]: 180.24
CAS: 139914-54-8

Physical Properties

Property code	Value	Unit	Source
gf	-133.66	kJ/mol	Joback Method
hf	-459.33	kJ/mol	Joback Method
hfus	15.38	kJ/mol	Joback Method
hvap	48.30	kJ/mol	Joback Method
ie	9.22	eV	NIST Webbook
log10ws	-1.81		Crippen Method
logp	1.827		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	603.67	K	Joback Method
tc	844.01	K	Joback Method
tf	367.01	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.77	J/mol×K	603.67	Joback Method
cpg	432.75	J/mol×K	643.73	Joback Method
cpg	452.52	J/mol×K	683.78	Joback Method
cpg	471.04	J/mol×K	723.84	Joback Method
cpg	488.29	J/mol×K	763.90	Joback Method
cpg	504.27	J/mol×K	803.96	Joback Method
cpg	518.93	J/mol×K	844.01	Joback Method

Sources

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=C139914548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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