6-Acetyl-5,8,8-trimethylbicyclo[3.2.1]octan-2,3-dio

Inchi: InChI=1S/C13H18O4/c1-7(14)17-10-5-8-11(16)9(15)6-13(10,4)12(8,2)3/h8,10H,5-6H2,1-
InchiKey: AZMIQLMLMLDESS-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CC(=O)OC1CC2C(=O)C(=O)CC1(C)C2(C)C
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-349.62	kJ/mol	Joback Method
hf	-708.77	kJ/mol	Joback Method
hfus	12.85	kJ/mol	Joback Method
hvap	59.43	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.512		Crippen Method
mcvol	182.890	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
ripol	2602.00		NIST Webbook
ripol	2602.00		NIST Webbook
tb	721.93	K	Joback Method
tc	964.74	K	Joback Method
tf	513.03	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.09	J/mol×K	721.93	Joback Method
cpg	577.26	J/mol×K	762.40	Joback Method
cpg	595.94	J/mol×K	802.87	Joback Method
cpg	614.34	J/mol×K	843.33	Joback Method
cpg	632.66	J/mol×K	883.80	Joback Method
cpg	651.13	J/mol×K	924.27	Joback Method

cpg	669.95	J/mol×K	964.74	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=R228883&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume