Bicyclo-2.2.1-heptane-2,3-dione,6-(acetyloxy)

Inchi: InChI=1S/C9H10O4/c1-4(10)13-7-3-5-2-6(7)9(12)8(5)11/h5-7H,2-3H2,1H3
InchiKey: JMULAZWICUTIIB-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: CC(=O)OC1CC2CC1C(=O)C2=O
Mol. weight [g/mol]: 182.17

Physical Properties

Property code	Value	Unit	Source
gf	-352.51	kJ/mol	Joback Method
hf	-630.19	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	52.97	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.096		Crippen Method
mcvol	126.530	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1684.00		NIST Webbook
tb	630.33	K	Joback Method
tc	867.40	K	Joback Method
tf	427.91	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.36	J/mol×K	630.33	Joback Method
cpg	367.62	J/mol×K	669.84	Joback Method
cpg	381.96	J/mol×K	709.35	Joback Method
cpg	395.37	J/mol×K	748.87	Joback Method
cpg	407.81	J/mol×K	788.38	Joback Method
cpg	419.28	J/mol×K	827.89	Joback Method
cpg	429.75	J/mol×K	867.40	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=R516279&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume