3-Oxabicyclo[3.2.1.]octane-2,4-dione, 6,7-dihydroxy-, 6,7-diacetate

Inchi: InChI=1S/C11H12O7/c1-4(12)16-8-6-3-7(9(8)17-5(2)13)11(15)18-10(6)14/h6-9H,3H2,1-2

InchiKey: RDFHBGLKBDMTEX-UHFFFAOYSA-N

Formula: C11H12O7

SMILES: CC(=O)OC1C2CC(C(=O)OC2=O)C1OC(C)=O

Mol. weight [g/mol]: 256.21

CAS: 13190-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-675.52	kJ/mol	Joback Method
hf	-1074.77	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	70.95	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	-0.431		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	778.93	K	Joback Method
tc	1013.29	K	Joback Method
tf	541.42	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.01	J/mol×K	778.93	Joback Method
cpg	547.45	J/mol×K	817.99	Joback Method
cpg	560.55	J/mol×K	857.05	Joback Method
cpg	572.23	J/mol×K	896.11	Joback Method
cpg	582.44	J/mol×K	935.17	Joback Method
cpg	591.13	J/mol×K	974.23	Joback Method
cpg	598.24	J/mol×K	1013.29	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=C13190777&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
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