D-Erythronic acid «gamma»-lactone, diacetate

Inchi: InChI=1S/C8H10O6/c1-4(9)13-6-3-12-8(11)7(6)14-5(2)10/h6-7H,3H2,1-2H3
InchiKey: KEHCWZIUXGQZOB-UHFFFAOYSA-N
Formula: C8H10O6
SMILES: CC(=O)OC1COC(=O)C1OC(C)=O
Mol. weight [g/mol]: 202.16

Physical Properties

Property code	Value	Unit	Source
gf	-631.23	kJ/mol	Joback Method
hf	-927.61	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	-0.593		Crippen Method
mcvol	135.040	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1445.50		NIST Webbook
tb	640.40	K	Joback Method
tc	862.18	K	Joback Method
tf	425.69	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.00	J/mol×K	640.40	Joback Method
cpg	377.28	J/mol×K	677.36	Joback Method
cpg	389.80	J/mol×K	714.33	Joback Method
cpg	401.51	J/mol×K	751.29	Joback Method
cpg	412.36	J/mol×K	788.25	Joback Method
cpg	422.31	J/mol×K	825.22	Joback Method
cpg	431.31	J/mol×K	862.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380075&Units=SI
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

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