Propanetricarboxylic acid, 1,2,3-, cyclic 1,2-anhydride

Inchi: InChI=1S/C6H6O5/c7-4(8)1-3-2-5(9)11-6(3)10/h3H,1-2H2,(H,7,8)
InchiKey: LYANEXCVXFZQFF-UHFFFAOYSA-N
Formula: C6H6O5
SMILES: O=C(O)CC1CC(=O)OC1=O
Mol. weight [g/mol]: 158.11
CAS: 4756-10-9

Physical Properties

Property code	Value	Unit	Source
gf	-560.85	kJ/mol	Joback Method
hf	-778.90	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.449		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
tb	660.60	K	Joback Method
tc	883.40	K	Joback Method
tf	442.04	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.03	J/mol×K	660.60	Joback Method
cpg	282.98	J/mol×K	697.73	Joback Method
cpg	292.31	J/mol×K	734.87	Joback Method
cpg	301.00	J/mol×K	772.00	Joback Method
cpg	309.00	J/mol×K	809.13	Joback Method
cpg	316.26	J/mol×K	846.26	Joback Method
cpg	322.75	J/mol×K	883.40	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=C4756109&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume