1,2,4-Cyclopentanetrione

Inchi: InChI=1S/C5H4O3/c6-3-1-4(7)5(8)2-3/h1-2H2
InchiKey: PLIKDTHMOISVIW-UHFFFAOYSA-N
Formula: C5H4O3
SMILES: O=C1CC(=O)C(=O)C1
Mol. weight [g/mol]: 112.08
CAS: 15849-14-6

Physical Properties

Property code	Value	Unit	Source
gf	-332.29	kJ/mol	Joback Method
hf	-478.81	kJ/mol	Joback Method
hfus	0.10	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	0.35		Crippen Method
logp	-0.512		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	537.21	K	Joback Method
tc	796.51	K	Joback Method
tf	365.91	K	Joback Method
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.47	J/mol×K	537.21	Joback Method
cpg	175.68	J/mol×K	580.43	Joback Method
cpg	186.57	J/mol×K	623.64	Joback Method
cpg	197.03	J/mol×K	666.86	Joback Method
cpg	206.94	J/mol×K	710.08	Joback Method
cpg	216.20	J/mol×K	753.30	Joback Method
cpg	224.70	J/mol×K	796.51	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=C15849146&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