1,2,4-Cyclopentanetrione, 3-methyl-

Other names: 3-Methyl-1,2,4-cyclopentanetrione
Inchi: InChI=1S/C6H6O3/c1-3-4(7)2-5(8)6(3)9/h3H,2H2,1H3
InchiKey: FUWXZDKUAHOVLL-UHFFFAOYSA-N
Formula: C6H6O3
SMILES: CC1C(=O)CC(=O)C1=O
Mol. weight [g/mol]: 126.11
CAS: 4505-54-8

Physical Properties

Property code	Value	Unit	Source
gf	-331.58	kJ/mol	Joback Method
hf	-519.79	kJ/mol	Joback Method
hfus	3.76	kJ/mol	Joback Method
hvap	41.95	kJ/mol	Joback Method
log10ws	0.17		Crippen Method
logp	-0.267		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	1090.00		NIST Webbook
tb	555.42	K	Joback Method
tc	809.08	K	Joback Method
tf	372.94	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.83	J/mol×K	555.42	Joback Method
cpg	222.94	J/mol×K	597.70	Joback Method
cpg	235.60	J/mol×K	639.97	Joback Method
cpg	247.69	J/mol×K	682.25	Joback Method
cpg	259.11	J/mol×K	724.53	Joback Method
cpg	269.75	J/mol×K	766.80	Joback Method
cpg	279.51	J/mol×K	809.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4505548&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

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