1,2-Cyclopentanedione, 3-methyl-

Other names: 3-Methyl-1,2-cyclopentanedione
3-Methylcyclopentane-1,2-dione
Inchi: InChI=1S/C6H8O2/c1-4-2-3-5(7)6(4)8/h4H,2-3H2,1H3
InchiKey: OACYKCIZDVVNJL-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1CCC(=O)C1=O
Mol. weight [g/mol]: 112.13
CAS: 765-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-208.99	kJ/mol	Joback Method
hf	-382.09	kJ/mol	Joback Method
hfus	4.25	kJ/mol	Joback Method
hvap	37.70	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.554		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
ripol	1781.00		NIST Webbook
tb	487.60	K	Joback Method
tc	724.67	K	Joback Method
tf	304.72	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.84	J/mol×K	487.60	Joback Method
cpg	201.89	J/mol×K	527.11	Joback Method
cpg	214.49	J/mol×K	566.62	Joback Method

cpg	226.61	J/mol×K	606.13	Joback Method
cpg	238.19	J/mol×K	645.64	Joback Method
cpg	249.18	J/mol×K	685.15	Joback Method
cpg	259.55	J/mol×K	724.67	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=C765708&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume