

3,5-Dimethyl-1,2-cyclopentanedione

Other names:	1,2-Cyclopentanedione, 3,5-dimethyl-3,5-dimethylcyclopentane-1,2-dione
Inchi:	InChI=1S/C7H10O2/c1-4-3-5(2)7(9)6(4)8/h4-5H,3H2,1-2H3
InchiKey:	MIDXCONKKJTLDX-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CC1CC(C)C(=O)C1=O
Mol. weight [g/mol]:	126.15
CAS:	13494-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-208.28	kJ/mol	Joback Method
hf	-423.07	kJ/mol	Joback Method
hfus	7.91	kJ/mol	Joback Method
hvap	39.62	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.801		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1044.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1769.00		NIST Webbook
tb	505.81	K	Joback Method
tc	738.45	K	Joback Method
tf	311.75	K	Joback Method
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.74	J/molxK	505.81	Joback Method
cpg	247.53	J/molxK	544.58	Joback Method
cpg	261.79	J/molxK	583.36	Joback Method
cpg	275.48	J/molxK	622.13	Joback Method

cpg	288.55	J/mol×K	660.90	Joback Method
cpg	300.94	J/mol×K	699.67	Joback Method
cpg	312.62	J/mol×K	738.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13494070&Units=SI

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

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