1-Cyclopentene-3,4-dione, 2,5-dimethyl

Inchi: InChI=1S/C7H8O2/c1-4-3-5(2)7(9)6(4)8/h3-4H,1-2H3
InchiKey: MIJHQCDCYTTZJR-UHFFFAOYSA-N
Formula: C7H8O2
SMILES: CC1=CC(C)C(=O)C1=O
Mol. weight [g/mol]: 124.14

Physical Properties

Property code	Value	Unit	Source
gf	-180.24	kJ/mol	Joback Method
hf	-356.42	kJ/mol	Joback Method
hfus	7.67	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.721		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1040.00		NIST Webbook
tb	514.62	K	Joback Method
tc	751.07	K	Joback Method
tf	329.27	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.96	J/mol×K	514.62	Joback Method
cpg	226.64	J/mol×K	554.03	Joback Method
cpg	238.88	J/mol×K	593.44	Joback Method
cpg	250.63	J/mol×K	632.85	Joback Method
cpg	261.85	J/mol×K	672.25	Joback Method
cpg	272.48	J/mol×K	711.66	Joback Method
cpg	282.47	J/mol×K	751.07	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87807&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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