1,3-Cyclohexanedione, 5,5-dimethyl-

Other names:	Cyclomethone
	Dimedon
	Dimedone
	Lu 274
	Medon
	Methon
	Methone
	1,1-Dimethyl-3,5-cyclohexanedione
	1,1-Dimethyl-3,5-diketocyclohexane
	5,5-Dimethyl-1,3-cyclohexanedione
	5,5-Dimethyldihydroresorcinol
	5,5-Dimethylhydroresorcinol
	5,5-Dimethylcyclohexane-1,3-dione
	5,5-Dimethyl-1,3-cyclohexadione
	5,5-Dimethyl-1,3-dihydroresorcinol
	NSC 14984
Inchi:	InChI=1S/C8H12O2/c1-8(2)4-6(9)3-7(10)5-8/h3-5H2,1-2H3
InchiKey:	BADXJIPKFRBFOT-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC1(C)CC(=O)CC(=O)C1
Mol. weight [g/mol]:	140.18
CAS:	126-81-8

Physical Properties

Property code	Value	Unit	Source
chs	-4379.70 ± 1.20	kJ/mol	NIST Webbook
gf	-209.74	kJ/mol	Joback Method
hf	-383.60 ± 1.90	kJ/mol	NIST Webbook
hfs	-483.40 ± 1.60	kJ/mol	NIST Webbook
hfus	1.03	kJ/mol	Joback Method
hsub	99.80 ± 1.10	kJ/mol	NIST Webbook
hsub	99.80 ± 1.10	kJ/mol	NIST Webbook
hvap	41.17	kJ/mol	Joback Method
ie	9.28 ± 0.05	eV	NIST Webbook
log10ws	-1.38		Crippen Method
logp	1.335		Crippen Method
mcvol	115.860	ml/mol	McGowan Method

pc	3602.88	kPa	Joback Method
rinpol	1101.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1101.00		NIST Webbook
tb	537.87	K	Joback Method
tc	785.42	K	Joback Method
tf	421.40 ± 3.00	K	NIST Webbook
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.77	J/mol×K	537.87	Joback Method
cpg	292.13	J/mol×K	579.13	Joback Method
cpg	307.63	J/mol×K	620.39	Joback Method
cpg	322.36	J/mol×K	661.64	Joback Method
cpg	336.38	J/mol×K	702.90	Joback Method
cpg	349.76	J/mol×K	744.16	Joback Method
cpg	362.57	J/mol×K	785.42	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126818&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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