1,3-Cyclohexanedione, 2,5,5-trimethyl-

Other names:	2-Methyldimedone
	2,5,5-Trimethyl-1,3-cyclohexanedione
Inchi:	InChI=1S/C9H14O2/c1-6-7(10)4-9(2,3)5-8(6)11/h6H,4-5H2,1-3H3
InchiKey:	WJTGLPHMQKJRIX-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC1C(=O)CC(C)(C)CC1=O
Mol. weight [g/mol]:	154.21
CAS:	1125-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-209.03	kJ/mol	Joback Method
hf	-455.27	kJ/mol	Joback Method
hfus	4.69	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Joback Method
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.581		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	556.08	K	Joback Method
tc	798.51	K	Joback Method
tf	354.67	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.74	J/mol×K	556.08	Joback Method
cpg	341.55	J/mol×K	596.48	Joback Method
cpg	358.48	J/mol×K	636.89	Joback Method
cpg	374.59	J/mol×K	677.29	Joback Method
cpg	389.95	J/mol×K	717.70	Joback Method
cpg	404.60	J/mol×K	758.10	Joback Method

cpg	418.61	J/mol×K	798.51	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=C1125117&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume