2,4-Hexanedione, 5,5-dimethyl-

Other names:	5,5-Dimethyl-hexan-2,4-dione
	5,5-Dimethylhexane-2,4-dione
	5,5-dimethyl-2,4-hexadione
	Pivaloylacetone, keto form
Inchi:	InChI=1S/C8H14O2/c1-6(9)5-7(10)8(2,3)4/h5H2,1-4H3
InchiKey:	LCLCVVVHIPPHCG-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(=O)CC(=O)C(C)(C)C
Mol. weight [g/mol]:	142.20
CAS:	7307-04-2

Physical Properties

Property code	Value	Unit	Source
gf	-238.52	kJ/mol	Joback Method
hf	-442.36	kJ/mol	Joback Method
hfus	12.26	kJ/mol	Joback Method
hvap	45.60	kJ/mol	Joback Method
log10ws	-1.63		Aqueous Solubility Prediction Method
logp	1.581		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	486.95	K	Joback Method
tc	684.39	K	Joback Method
tf	282.20	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.31	J/mol×K	486.95	Joback Method
cpg	291.11	J/mol×K	519.86	Joback Method
cpg	303.20	J/mol×K	552.76	Joback Method
cpg	314.60	J/mol×K	585.67	Joback Method

cpg	325.33	J/mol×K	618.58	Joback Method
cpg	335.44	J/mol×K	651.49	Joback Method
cpg	344.96	J/mol×K	684.39	Joback Method
dvisc	0.0047661	Pa×s	282.20	Joback Method
dvisc	0.0023982	Pa×s	316.33	Joback Method
dvisc	0.0013794	Pa×s	350.45	Joback Method
dvisc	0.0008752	Pa×s	384.58	Joback Method
dvisc	0.0005981	Pa×s	418.70	Joback Method
dvisc	0.0004328	Pa×s	452.83	Joback Method
dvisc	0.0003278	Pa×s	486.95	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7307042&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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