Pivaloylacetone, keto form

Other names: 5,5-Dimethyl-hexan-2,4-dione
5,5-Dimethylhexane-2,4-dione
5,5-dimethyl-2,4-hexadione
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

Physical Properties

Property code	Value	Unit	Source
hf	-460.70	kJ/mol	Cheméo Relay (1.0)
hfus	12.26	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-1.63		Aqueous Solubility Prediction Method
logp	1.581		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
tb	457.65	K	Cheméo Relay (1.0)
tc	635.00	K	Cheméo Relay (1.0)
tf	284.04	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7307042&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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