2,2-Dimethylheptane-3,5-dione

Other names: 2,2-Dimethyl-3,5-heptanedione
Pivaloylpropionylmethane
6,6-Dimethyl-3,5-heptanedione
Inchi: InChI=1S/C9H16O2/c1-5-7(10)6-8(11)9(2,3)4/h5-6H2,1-4H3
InchiKey: LHQYNVWJWUCTSS-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCC(=O)CC(=O)C(C)(C)C
Mol. weight [g/mol]: 156.22
CAS: 20734-29-6

Physical Properties

Property code	Value	Unit	Source
chl	-5301.10 ± 1.80	kJ/mol	NIST Webbook
gf	-230.10	kJ/mol	Joback Method
hf	-470.90 ± 2.30	kJ/mol	NIST Webbook
hfl	-527.10 ± 2.20	kJ/mol	NIST Webbook
hfl	-527.80 ± 2.30	kJ/mol	NIST Webbook
hfus	14.85	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.971		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	509.83	K	Joback Method
tc	704.75	K	Joback Method
tf	293.47	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.25	J/mol×K	509.83	Joback Method
cpg	383.51	J/mol×K	672.27	Joback Method
cpg	372.64	J/mol×K	639.78	Joback Method

cpg	361.11	J/mol×K	607.29	Joback Method
cpg	348.89	J/mol×K	574.80	Joback Method
cpg	335.95	J/mol×K	542.32	Joback Method
cpg	393.74	J/mol×K	704.75	Joback Method
dvisc	0.0003008	Pa×s	509.83	Joback Method
dvisc	0.0003989	Pa×s	473.77	Joback Method
dvisc	0.0005542	Pa×s	437.71	Joback Method
dvisc	0.0008168	Pa×s	401.65	Joback Method
dvisc	0.0012995	Pa×s	365.59	Joback Method
dvisc	0.0022886	Pa×s	329.53	Joback Method
dvisc	0.0046319	Pa×s	293.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20734296&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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