3,5-Heptanedione, 2,6-dimethyl-

Other names: 2,6-Dimethyl-3,5-heptanedione
2,6-dimethylheptane-3,5-dione
Inchi: InChI=1S/C9H16O2/c1-6(2)8(10)5-9(11)7(3)4/h6-7H,5H2,1-4H3
InchiKey: CEGGECULKVTYMM-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC(C)C(=O)CC(=O)C(C)C
Mol. weight [g/mol]: 156.22
CAS: 18362-64-6

Physical Properties

Property code	Value	Unit	Source
chl	-5301.40 ± 1.60	kJ/mol	NIST Webbook
gf	-237.82	kJ/mol	Joback Method
hf	-470.40 ± 2.10	kJ/mol	NIST Webbook
hfl	-526.80 ± 2.00	kJ/mol	NIST Webbook
hfl	-527.30 ± 2.10	kJ/mol	NIST Webbook
hfus	15.22	kJ/mol	Joback Method
hvap	56.10	kJ/mol	NIST Webbook
log10ws	-1.67		Crippen Method
logp	1.827		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	512.18	K	Joback Method
tc	703.77	K	Joback Method
tf	261.05	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.58	J/mol×K	512.18	Joback Method

cpg	332.99	J/mol×K	544.11	Joback Method
cpg	345.76	J/mol×K	576.04	Joback Method
cpg	357.91	J/mol×K	607.98	Joback Method
cpg	369.47	J/mol×K	639.91	Joback Method
cpg	380.44	J/mol×K	671.84	Joback Method
cpg	390.83	J/mol×K	703.77	Joback Method
dvisc	0.0071523	Pa×s	261.05	Joback Method
dvisc	0.0028688	Pa×s	302.91	Joback Method
dvisc	0.0014364	Pa×s	344.76	Joback Method
dvisc	0.0008354	Pa×s	386.62	Joback Method
dvisc	0.0005402	Pa×s	428.47	Joback Method
dvisc	0.0003774	Pa×s	470.33	Joback Method
dvisc	0.0002796	Pa×s	512.18	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18362646&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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