3,5-Heptanedione, 2,2,6-trimethyl-

Other names: 2,2,6-trimethylheptane-3,5-dione
Inchi: InChI=1S/C10H18O2/c1-7(2)8(11)6-9(12)10(3,4)5/h7H,6H2,1-5H3
InchiKey: KLKRGCUPZROPPO-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)C(=O)CC(=O)C(C)(C)C
Mol. weight [g/mol]: 170.25
CAS: 7333-23-5

Physical Properties

Property code	Value	Unit	Source
chl	-5939.50 ± 1.50	kJ/mol	NIST Webbook
gf	-224.12	kJ/mol	Joback Method
hf	-510.70 ± 2.10	kJ/mol	NIST Webbook
hfl	-568.40 ± 2.10	kJ/mol	NIST Webbook
hfl	-568.10 ± 2.00	kJ/mol	NIST Webbook
hfus	13.92	kJ/mol	Joback Method
hvap	57.70	kJ/mol	NIST Webbook
log10ws	-2.09		Crippen Method
logp	2.217		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	532.27	K	Joback Method
tc	728.77	K	Joback Method
tf	289.74	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.32	J/mol×K	532.27	Joback Method
cpg	434.64	J/mol×K	696.02	Joback Method
cpg	422.89	J/mol×K	663.27	Joback Method
cpg	410.42	J/mol×K	630.52	Joback Method
cpg	397.19	J/mol×K	597.77	Joback Method

cpg	383.17	J/mol×K	565.02	Joback Method
cpg	445.70	J/mol×K	728.77	Joback Method
dvisc	0.0002575	Pa×s	532.27	Joback Method
dvisc	0.0003519	Pa×s	491.85	Joback Method
dvisc	0.0005086	Pa×s	451.43	Joback Method
dvisc	0.0007902	Pa×s	411.00	Joback Method
dvisc	0.0013518	Pa×s	370.58	Joback Method
dvisc	0.0026371	Pa×s	330.16	Joback Method
dvisc	0.0061991	Pa×s	289.74	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=C7333235&Units=SI

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

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