3,5-Octanedione, 2,7-dimethyl-

Other names: 2,7-Dimethyloctane-3,5-dione
Inchi: InChI=1S/C10H18O2/c1-7(2)5-9(11)6-10(12)8(3)4/h7-8H,5-6H2,1-4H3
InchiKey: QVXCBARKVVWYOM-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)CC(=O)CC(=O)C(C)C
Mol. weight [g/mol]: 170.25
CAS: 7307-07-5

Physical Properties

Property code	Value	Unit	Source
gf	-229.40	kJ/mol	Joback Method
hf	-485.45	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	50.57	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.217		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1165.20		NIST Webbook
rinpol	1165.20		NIST Webbook
tb	535.06	K	Joback Method
tc	724.34	K	Joback Method
tf	272.32	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.42	J/mol×K	535.06	Joback Method
cpg	379.67	J/mol×K	566.61	Joback Method
cpg	393.24	J/mol×K	598.15	Joback Method
cpg	406.15	J/mol×K	629.70	Joback Method
cpg	418.43	J/mol×K	661.25	Joback Method
cpg	430.08	J/mol×K	692.79	Joback Method

cpg	441.12	J/mol×K	724.34	Joback Method
dvisc	0.0068659	Pa×s	272.32	Joback Method
dvisc	0.0027202	Pa×s	316.11	Joback Method
dvisc	0.0013501	Pa×s	359.90	Joback Method
dvisc	0.0007800	Pa×s	403.69	Joback Method
dvisc	0.0005018	Pa×s	447.48	Joback Method
dvisc	0.0003492	Pa×s	491.27	Joback Method
dvisc	0.0002579	Pa×s	535.06	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=C7307075&Units=SI

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
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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