3,5-Heptanedione, 2,2,6,6-tetramethyl-

Other names:	Dipivaloylmethane
	2,2,6,6-Tetramethyl-3,5-heptanedione
	(CH3)3CCOCH2COC(CH3)3
	2,2,6,6-Tetramethylheptane-3,5-dione
	2,2,6,6-Tetramethyl heptanedione
Inchi:	InChI=1S/C11H20O2/c1-10(2,3)8(12)7-9(13)11(4,5)6/h7H2,1-6H3
InchiKey:	YRAJNWYBUCUFBD-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CC(C)(C)C(=O)CC(=O)C(C)(C)C
Mol. weight [g/mol]:	184.28
CAS:	1118-71-4

Physical Properties

Property code	Value	Unit	Source
chl	-6599.20 ± 3.50	kJ/mol	NIST Webbook
gf	-210.42	kJ/mol	Joback Method
hf	-528.40 ± 3.90	kJ/mol	NIST Webbook
hfl	-587.70 ± 3.80	kJ/mol	NIST Webbook
hfl	-587.90 ± 3.90	kJ/mol	NIST Webbook
hfus	12.62	kJ/mol	Joback Method
hvap	59.54	kJ/mol	NIST Webbook
hvap	59.50	kJ/mol	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	8.86 ± 0.07	eV	NIST Webbook
log10ws	-2.50		Crippen Method
logp	2.607		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	552.36	K	Joback Method
tc	753.62	K	Joback Method
tf	318.43	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.71	J/mol×K	552.36	Joback Method
cpg	434.83	J/mol×K	585.90	Joback Method
cpg	449.93	J/mol×K	619.45	Joback Method
cpg	464.08	J/mol×K	652.99	Joback Method
cpg	477.33	J/mol×K	686.54	Joback Method
cpg	489.74	J/mol×K	720.08	Joback Method
cpg	501.36	J/mol×K	753.62	Joback Method
dvisc	0.0049922	Pa×s	318.43	Joback Method
dvisc	0.0022552	Pa×s	357.42	Joback Method
dvisc	0.0011912	Pa×s	396.41	Joback Method
dvisc	0.0007053	Pa×s	435.39	Joback Method
dvisc	0.0004552	Pa×s	474.38	Joback Method
dvisc	0.0003140	Pa×s	513.37	Joback Method
dvisc	0.0002283	Pa×s	552.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.70	K	0.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1118714&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

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

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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume