Pentanoic acid, 4,4-dimethyl-3-oxo-, methyl ester

Other names: Methyl 4,4-dimethyl-3-oxovalerate
Methyl 4,4-dimethyl-3-oxopentanoate
Methyl pivaloylacetate
Methyl 4,4,4-trimethyl-3-oxobutanoate
Methyl 3-oxo-4,4-dimethylpentanoate

Inchi: InChI=1S/C8H14O3/c1-8(2,3)6(9)5-7(10)11-4/h5H2,1-4H3

InchiKey: XTXCFTMJPRXBBC-UHFFFAOYSA-N

Formula: C8H14O3

SMILES: COC(=O)CC(=O)C(C)(C)C

Mol. weight [g/mol]: 158.19

CAS: 55107-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-343.52	kJ/mol	Joback Method
hf	-574.58	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.165		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	509.37	K	Joback Method
tc	705.37	K	Joback Method
tf	304.43	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.98	J/mol×K	509.37	Joback Method
cpg	314.46	J/mol×K	542.04	Joback Method
cpg	326.31	J/mol×K	574.70	Joback Method
cpg	337.53	J/mol×K	607.37	Joback Method

cpg	348.15	J/mol×K	640.04	Joback Method
cpg	358.18	J/mol×K	672.71	Joback Method
cpg	367.64	J/mol×K	705.37	Joback Method
dvisc	0.0033814	Pa×s	304.43	Joback Method
dvisc	0.0017905	Pa×s	338.59	Joback Method
dvisc	0.0010652	Pa×s	372.74	Joback Method
dvisc	0.0006915	Pa×s	406.90	Joback Method
dvisc	0.0004799	Pa×s	441.06	Joback Method
dvisc	0.0003511	Pa×s	475.21	Joback Method
dvisc	0.0002678	Pa×s	509.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.70	K	1.70	NIST Webbook

Sources

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=C55107147&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume