Butanoic acid, 2,2-dimethyl-3-oxo-, methyl ester

Other names: 2,2-Dimethyl-3-oxobutyric acid, methyl ester
Acetoacetic acid, 2,2-dimethyl-, methyl ester
methyl 2,2-dimethylacetoacetate

Inchi: InChI=1S/C7H12O3/c1-5(8)7(2,3)6(9)10-4/h1-4H3

InchiKey: LVSDLZIEHYYLTC-UHFFFAOYSA-N

Formula: C7H12O3

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

Mol. weight [g/mol]: 144.17

CAS: 38923-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-351.94	kJ/mol	Joback Method
hf	-553.94	kJ/mol	Joback Method
hfus	10.86	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.775		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	486.49	K	Joback Method
tc	685.06	K	Joback Method
tf	293.16	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.04	J/mol×K	486.49	Joback Method
cpg	270.52	J/mol×K	519.59	Joback Method
cpg	281.41	J/mol×K	552.68	Joback Method
cpg	291.72	J/mol×K	585.78	Joback Method
cpg	301.47	J/mol×K	618.87	Joback Method
cpg	310.68	J/mol×K	651.97	Joback Method

cpg	319.36	J/mol×K	685.06	Joback Method
dvisc	0.0034748	Pa×s	293.16	Joback Method
dvisc	0.0018762	Pa×s	325.38	Joback Method
dvisc	0.0011320	Pa×s	357.60	Joback Method
dvisc	0.0007425	Pa×s	389.83	Joback Method
dvisc	0.0005194	Pa×s	422.05	Joback Method
dvisc	0.0003822	Pa×s	454.27	Joback Method
dvisc	0.0002929	Pa×s	486.49	Joback Method

Sources

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=C38923578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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