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

Other names:	Acetoacetic acid, 2-methyl-, ethyl ester
	«alpha»-Methylacetoacetic ester
	Ethyl «alpha»-acetylpropionate
	Ethyl «alpha»-methylacetoacetate
	Ethyl «alpha»-methylacetylacetate
	Ethyl 2-acetylpropionate
	Ethyl 2-methyl-3-oxobutanoate
	Ethyl 2-methyl-3-oxobutyrate
	Ethyl 2-methylacetoacetate
	Ethyl methylacetoacetate
	2-Methylacetoacetic acid ethyl ester
	Ethyl ester of 2-methyl-3-oxobutanoic acid
	2-Methyl-3-oxobutanoic acid ethyl ester
	NSC 1102
Inchi:	InChI=1S/C7H12O3/c1-4-10-7(9)5(2)6(3)8/h5H,4H2,1-3H3
InchiKey:	FNENWZWNOPCZGK-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CCOC(=O)C(C)C(C)=O
Mol. weight [g/mol]:	144.17
CAS:	609-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-357.22	kJ/mol	Joback Method
hf	-550.47	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	46.69	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.775		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	460.20	K	NIST Webbook
tc	680.12	K	Joback Method
tf	275.74	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.03	J/mol×K	489.28	Joback Method
cpg	266.86	J/mol×K	521.09	Joback Method
cpg	277.26	J/mol×K	552.89	Joback Method
cpg	287.23	J/mol×K	584.70	Joback Method
cpg	296.77	J/mol×K	616.51	Joback Method
cpg	305.87	J/mol×K	648.32	Joback Method
cpg	314.54	J/mol×K	680.12	Joback Method
dvisc	0.0036824	Pa×s	275.74	Joback Method
dvisc	0.0018798	Pa×s	311.33	Joback Method
dvisc	0.0011016	Pa×s	346.92	Joback Method
dvisc	0.0007130	Pa×s	382.51	Joback Method
dvisc	0.0004970	Pa×s	418.10	Joback Method
dvisc	0.0003666	Pa×s	453.69	Joback Method
dvisc	0.0002827	Pa×s	489.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609143&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

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

Latest version available from:
https://www.chemeo.com/cid/52-992-3/Butanoic-acid-2-methyl-3-oxo-ethyl-ester.pdf
Generated by Cheméo on 2024-04-18 06:17:51.532607221 +0000 UTC m=+15710320.453184554.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.