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

Other names:	Acetoacetic acid, 2-isopropyl-, ethyl ester
	Ethyl «alpha»-isopropylacetoacetate
	Ethyl 2-acetyl-3-methylbutanoate
	Ethyl 2-isopropylacetoacetate
	2-Isopropylacetoacetic acid ethyl ester
	ethyl 2-acetyl-3-methylbutyrate
Inchi:	InChI=1S/C9H16O3/c1-5-12-9(11)8(6(2)3)7(4)10/h6,8H,5H2,1-4H3
InchiKey:	DMIFFKCVURTPTG-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CCOC(=O)C(C(C)=O)C(C)C
Mol. weight [g/mol]:	172.22
CAS:	1522-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-342.82	kJ/mol	Joback Method
hf	-597.03	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.411		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	534.60	K	Joback Method
tc	724.87	K	Joback Method
tf	283.28	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.13	J/mol×K	534.60	Joback Method
cpg	357.29	J/mol×K	566.31	Joback Method
cpg	369.87	J/mol×K	598.02	Joback Method

cpg	381.89	J/mol×K	629.74	Joback Method
cpg	393.33	J/mol×K	661.45	Joback Method
cpg	404.21	J/mol×K	693.16	Joback Method
cpg	414.54	J/mol×K	724.87	Joback Method
dvisc	0.0049091	Pa×s	283.28	Joback Method
dvisc	0.0021186	Pa×s	325.17	Joback Method
dvisc	0.0011076	Pa×s	367.05	Joback Method
dvisc	0.0006613	Pa×s	408.94	Joback Method
dvisc	0.0004346	Pa×s	450.83	Joback Method
dvisc	0.0003067	Pa×s	492.71	Joback Method
dvisc	0.0002286	Pa×s	534.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	2.70	NIST Webbook
tbrp	369.50 ± 0.50	K	2.70	NIST Webbook

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=C1522469&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume