Ethyl 2-acetylbutyrate

Other names:	Butanoic acid, 2-ethyl-3-oxo-, ethyl ester
	Acetoacetic acid, 2-ethyl-, ethyl ester
	Ethyl «alpha»-acetylbutyrate
	Ethyl «alpha»-ethylacetoacetate
	Ethyl 2-ethyl-3-ketobutyrate
	Ethyl 2-ethylacetoacetate
	2-Ethyl-3-oxobutanoic acid ethyl ester
	Ethyl ethylacetoacetate
	NSC 53775
	2-Ethylacetoacetic acid ethyl ester
Inchi:	InChI=1S/C8H14O3/c1-4-7(6(3)9)8(10)11-5-2/h7H,4-5H2,1-3H3
InchiKey:	OKANYBNORCUPKZ-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCOC(=O)C(CC)C(C)=O
Mol. weight [g/mol]:	158.19
CAS:	607-97-6

Physical Properties

Property code	Value	Unit	Source
chl	-4432.30 ± 2.10	kJ/mol	NIST Webbook
gf	-348.80	kJ/mol	Joback Method
hf	-571.11	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.165		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	471.15 ± 1.00	K	NIST Webbook
tc	700.78	K	Joback Method
tf	287.01	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.98	J/mol×K	700.78	Joback Method
cpg	298.94	J/mol×K	512.16	Joback Method
cpg	310.84	J/mol×K	543.60	Joback Method
cpg	322.24	J/mol×K	575.03	Joback Method
cpg	333.16	J/mol×K	606.47	Joback Method
cpg	343.58	J/mol×K	637.91	Joback Method
cpg	353.52	J/mol×K	669.35	Joback Method
dvisc	0.0002635	Pa×s	512.16	Joback Method
dvisc	0.0036492	Pa×s	287.01	Joback Method
dvisc	0.0018279	Pa×s	324.53	Joback Method
dvisc	0.0010567	Pa×s	362.06	Joback Method
dvisc	0.0006771	Pa×s	399.58	Joback Method
dvisc	0.0004683	Pa×s	437.11	Joback Method
dvisc	0.0003434	Pa×s	474.63	Joback Method
hvapt	53.30	kJ/mol	392.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607976&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

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
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
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