Ethyl diacetoacetate

Other names:	Butanoic acid, 2-acetyl-3-oxo-, ethyl ester
	Acetoacetic acid, 2-acetyl-, ethyl ester
	Ethyl diacetylacetate
	Ethyl 2-acetylacetoacetate
Inchi:	InChI=1S/C8H12O4/c1-4-12-8(11)7(5(2)9)6(3)10/h7H,4H2,1-3H3
InchiKey:	YMCDYRGMTRCAPZ-UHFFFAOYSA-N
Formula:	C8H12O4
SMILES:	CCOC(=O)C(C(C)=O)C(C)=O
Mol. weight [g/mol]:	172.18
CAS:	603-69-0

Physical Properties

Property code	Value	Unit	Source
chl	-4073.50	kJ/mol	NIST Webbook
gf	-477.72	kJ/mol	Joback Method
hf	-683.69	kJ/mol	Joback Method
hfl	-789.50	kJ/mol	NIST Webbook
hfus	18.94	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.344		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	566.03	K	Joback Method
tc	763.18	K	Joback Method
tf	336.94	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.89	J/mol×K	566.03	Joback Method
cpg	325.92	J/mol×K	598.89	Joback Method
cpg	336.43	J/mol×K	631.75	Joback Method

cpg	346.41	J/mol×K	664.60	Joback Method
cpg	355.86	J/mol×K	697.46	Joback Method
cpg	364.79	J/mol×K	730.32	Joback Method
cpg	373.18	J/mol×K	763.18	Joback Method
dvisc	0.0029238	Pa×s	336.94	Joback Method
dvisc	0.0016163	Pa×s	375.12	Joback Method
dvisc	0.0009969	Pa×s	413.30	Joback Method
dvisc	0.0006672	Pa×s	451.49	Joback Method
dvisc	0.0004755	Pa×s	489.67	Joback Method
dvisc	0.0003558	Pa×s	527.85	Joback Method
dvisc	0.0002769	Pa×s	566.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	2.10	NIST Webbook
tbrp	377.00	K	2.10	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=C603690&Units=SI

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
hfl: Liquid phase 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