Hexanoic acid, 2-acetyl-5-oxo-, ethyl ester

Inchi: InChI=1S/C10H16O4/c1-4-14-10(13)9(8(3)12)6-5-7(2)11/h9H,4-6H2,1-3H3
InchiKey: FSXQBIOXTYIIDI-UHFFFAOYSA-N
Formula: C10H16O4
SMILES: CCOC(=O)C(CCC(C)=O)C(C)=O
Mol. weight [g/mol]: 200.23
CAS: 35490-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-460.88	kJ/mol	Joback Method
hf	-724.97	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.124		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
tb	611.79	K	Joback Method
tc	803.96	K	Joback Method
tf	359.48	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.26	J/mol×K	611.79	Joback Method
cpg	466.30	J/mol×K	771.93	Joback Method
cpg	456.13	J/mol×K	739.90	Joback Method
cpg	445.35	J/mol×K	707.88	Joback Method
cpg	433.95	J/mol×K	675.85	Joback Method
cpg	421.92	J/mol×K	643.82	Joback Method
cpg	475.85	J/mol×K	803.96	Joback Method
dvisc	0.0002270	Pa×s	611.79	Joback Method
dvisc	0.0002943	Pa×s	569.74	Joback Method

dvisc	0.0003976	Pa×s	527.69	Joback Method
dvisc	0.0005658	Pa×s	485.63	Joback Method
dvisc	0.0008610	Pa×s	443.58	Joback Method
dvisc	0.0014305	Pa×s	401.53	Joback Method
dvisc	0.0026766	Pa×s	359.48	Joback Method

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=C35490052&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume