ethyl 2-acetoxypropanoate

Inchi: InChI=1S/C7H12O4/c1-4-10-7(9)5(2)11-6(3)8/h5H,4H2,1-3H3
InchiKey: BCHOKJRLDTXCSF-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: CCOC(=O)C(C)OC(C)=O
Mol. weight [g/mol]: 160.17

Physical Properties

Property code	Value	Unit	Source
gf	-462.22	kJ/mol	Joback Method
hf	-682.69	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.501		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook
tb	511.70	K	Joback Method
tc	701.34	K	Joback Method
tf	297.97	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.59	J/mol×K	511.70	Joback Method
cpg	328.25	J/mol×K	669.73	Joback Method
cpg	319.13	J/mol×K	638.13	Joback Method
cpg	309.59	J/mol×K	606.52	Joback Method
cpg	299.65	J/mol×K	574.91	Joback Method
cpg	289.32	J/mol×K	543.31	Joback Method
cpg	336.95	J/mol×K	701.34	Joback Method
dvisc	0.0002344	Pa×s	511.70	Joback Method

dvisc	0.0003024	Pa×s	476.08	Joback Method
dvisc	0.0004067	Pa×s	440.46	Joback Method
dvisc	0.0005762	Pa×s	404.84	Joback Method
dvisc	0.0008732	Pa×s	369.21	Joback Method
dvisc	0.0014459	Pa×s	333.59	Joback Method
dvisc	0.0027013	Pa×s	297.97	Joback Method

Sources

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=R332724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume