ETHYL (+-)-3-ACETOXYBUTYRATE

Other names: Ethyl 3-(acetyloxy)butanoate
Ethyl 3-acetoxybutanoate
Butyric acid, 3-hydroxy-, ethyl ester, acetate
Inchi: InChI=1S/C8H14O4/c1-4-11-8(10)5-6(2)12-7(3)9/h6H,4-5H2,1-3H3
InchiKey: JFWYJXYRFBRWSH-UHFFFAOYSA-N
Formula: C8H14O4
SMILES: CCOC(=O)CC(C)OC(C)=O
Mol. weight [g/mol]: 174.20

Physical Properties

Property code	Value	Unit	Source
af	0.5488		Cheméo Relay (1.0)
gf	-453.80	kJ/mol	Joback Method
hf	-874.24	kJ/mol	Cheméo Relay (1.0)
hfus	18.53	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-0.85		Cheméo Relay (1.0)
logp	0.891		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	446.97	K	Cheméo Relay (1.0)
tc	630.92	K	Cheméo Relay (1.0)
tf	234.18	K	Cheméo Relay (1.0)
vc	0.526	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.54	J/mol×K	534.58	Joback Method
cpg	386.20	J/mol×K	722.01	Joback Method
cpg	376.76	J/mol×K	690.77	Joback Method
cpg	366.85	J/mol×K	659.53	Joback Method
cpg	356.46	J/mol×K	628.29	Joback Method

cpg	345.61	J/mol×K	597.06	Joback Method
cpg	334.30	J/mol×K	565.82	Joback Method
dvisc	0.0005393	Pa×s	421.91	Joback Method
dvisc	0.0002153	Pa×s	534.58	Joback Method
dvisc	0.0002792	Pa×s	497.02	Joback Method
dvisc	0.0003777	Pa×s	459.47	Joback Method
dvisc	0.0026376	Pa×s	309.24	Joback Method
dvisc	0.0008255	Pa×s	384.35	Joback Method
dvisc	0.0013856	Pa×s	346.80	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27846497&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie: Ionization energy
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