ethyl 3-hydroxyoctanoate

Inchi: InChI=1S/C10H20O3/c1-3-5-6-7-9(11)8-10(12)13-4-2/h9,11H,3-8H2,1-2H3
InchiKey: VGWUJHSTGYCXQQ-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]: 188.26
CAS: 7367-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-339.86	kJ/mol	Joback Method
hf	-652.04	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.881		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
ripol	1874.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1886.00		NIST Webbook
tb	596.23	K	Joback Method
tc	765.82	K	Joback Method
tf	320.44	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/mol×K	596.23	Joback Method
cpg	441.47	J/mol×K	624.50	Joback Method
cpg	453.52	J/mol×K	652.76	Joback Method
cpg	465.05	J/mol×K	681.03	Joback Method
cpg	476.07	J/mol×K	709.29	Joback Method
cpg	486.60	J/mol×K	737.56	Joback Method
cpg	496.65	J/mol×K	765.82	Joback Method
dvisc	0.0094549	Pa×s	320.44	Joback Method
dvisc	0.0025198	Pa×s	366.41	Joback Method
dvisc	0.0009018	Pa×s	412.37	Joback Method
dvisc	0.0003966	Pa×s	458.34	Joback Method
dvisc	0.0002026	Pa×s	504.30	Joback Method
dvisc	0.0001158	Pa×s	550.27	Joback Method
dvisc	0.0000721	Pa×s	596.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7367900&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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