

Ethyl 3-hydroxyhexadecanoate

Inchi:	InChI=1S/C18H36O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-17(19)16-18(20)21-4-2/h17,19H
InchiKey:	LTSBJVJXSJSRRZ-UHFFFAOYSA-N
Formula:	C18H36O3
SMILES:	CCCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]:	300.48
CAS:	105918-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-272.50	kJ/mol	Joback Method
hf	-817.16	kJ/mol	Joback Method
hfus	45.73	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.002		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2142.30		NIST Webbook
rinpol	2142.30		NIST Webbook
tb	779.27	K	Joback Method
tc	956.35	K	Joback Method
tf	410.60	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.00	J/mol×K	779.27	Joback Method
cpg	884.08	J/mol×K	808.78	Joback Method
cpg	900.29	J/mol×K	838.30	Joback Method
cpg	915.65	J/mol×K	867.81	Joback Method
cpg	930.20	J/mol×K	897.33	Joback Method
cpg	943.94	J/mol×K	926.84	Joback Method
cpg	956.90	J/mol×K	956.35	Joback Method

dvisc	0.0019004	Paxs	410.60	Joback Method
dvisc	0.0005130	Paxs	472.05	Joback Method
dvisc	0.0001872	Paxs	533.49	Joback Method
dvisc	0.0000841	Paxs	594.93	Joback Method
dvisc	0.0000439	Paxs	656.38	Joback Method
dvisc	0.0000256	Paxs	717.83	Joback Method
dvisc	0.0000163	Paxs	779.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C105918272&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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