

Ethyl 3-hydroxyoctadecanoate

Inchi:	InChI=1S/C20H40O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19(21)18-20(22)23-4-2/h
InchiKey:	BXRPWBZYLZSTNL-UHFFFAOYSA-N
Formula:	C20H40O3
SMILES:	CCCCCCCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]:	328.53
CAS:	65144-03-8

Physical Properties

Property code	Value	Unit	Source
gf	-255.66	kJ/mol	Joback Method
hf	-858.44	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	85.56	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.782		Crippen Method
mcvol	305.970	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2347.90		NIST Webbook
rinpol	2347.90		NIST Webbook
tb	825.03	K	Joback Method
tc	1010.12	K	Joback Method
tf	433.14	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.35	J/molxK	825.03	Joback Method
cpg	1068.70	J/molxK	979.27	Joback Method
cpg	1054.31	J/molxK	948.42	Joback Method
cpg	1039.01	J/molxK	917.58	Joback Method
cpg	1022.77	J/molxK	886.73	Joback Method
cpg	1005.56	J/molxK	855.88	Joback Method
cpg	1082.21	J/molxK	1010.12	Joback Method

dvisc	0.0000112	Paxs	825.03	Joback Method
dvisc	0.0000176	Paxs	759.71	Joback Method
dvisc	0.0000300	Paxs	694.40	Joback Method
dvisc	0.0000572	Paxs	629.09	Joback Method
dvisc	0.0001267	Paxs	563.77	Joback Method
dvisc	0.0003457	Paxs	498.45	Joback Method
dvisc	0.0012770	Paxs	433.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C65144038&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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