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/h1
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/mol×K	825.03	Joback Method
cpg	1005.56	J/mol×K	855.88	Joback Method
cpg	1022.77	J/mol×K	886.73	Joback Method
cpg	1039.01	J/mol×K	917.58	Joback Method
cpg	1054.31	J/mol×K	948.42	Joback Method
cpg	1068.70	J/mol×K	979.27	Joback Method
cpg	1082.21	J/mol×K	1010.12	Joback Method

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65144038&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

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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