Tridecanoic acid, 3-hydroxy-, ethyl ester

Inchi: InChI=1S/C15H30O3/c1-3-5-6-7-8-9-10-11-12-14(16)13-15(17)18-4-2/h14,16H,3-13H2,1
InchiKey: LOFDGMSAUOHYLH-UHFFFAOYSA-N
Formula: C15H30O3
SMILES: CCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]: 258.40
CAS: 107141-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-297.76	kJ/mol	Joback Method
hf	-755.24	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.831		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
ripol	2433.00		NIST Webbook
tb	710.63	K	Joback Method
tc	881.04	K	Joback Method
tf	376.79	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.58	J/mol×K	710.63	Joback Method
cpg	709.09	J/mol×K	739.03	Joback Method
cpg	723.89	J/mol×K	767.43	Joback Method
cpg	737.97	J/mol×K	795.83	Joback Method
cpg	751.37	J/mol×K	824.23	Joback Method
cpg	764.10	J/mol×K	852.63	Joback Method
cpg	776.17	J/mol×K	881.04	Joback Method
dvisc	0.0034600	Pa×s	376.79	Joback Method

dvisc	0.0009296	Pa×s	432.43	Joback Method
dvisc	0.0003370	Pa×s	488.07	Joback Method
dvisc	0.0001504	Pa×s	543.71	Joback Method
dvisc	0.0000780	Pa×s	599.35	Joback Method
dvisc	0.0000452	Pa×s	654.99	Joback Method
dvisc	0.0000285	Pa×s	710.63	Joback Method

Sources

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=C107141151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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