Ethyl 3-hydroxyicosanoate

Inchi: InChI=1S/C22H44O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(23)20-22(24)25
InchiKey: DRMKUFKWLLRFLJ-UHFFFAOYSA-N
Formula: C22H44O3
SMILES: CCCCCCCCCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]: 356.58

Physical Properties

Property code	Value	Unit	Source
gf	-238.82	kJ/mol	Joback Method
hf	-899.72	kJ/mol	Joback Method
hfus	56.09	kJ/mol	Joback Method
hvap	90.01	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.562		Crippen Method
mcvol	334.150	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2551.40		NIST Webbook
rinpol	2551.40		NIST Webbook
tb	870.79	K	Joback Method
tc	1067.36	K	Joback Method
tf	455.68	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.85	J/mol×K	870.79	Joback Method
cpg	1196.98	J/mol×K	1034.60	Joback Method
cpg	1181.93	J/mol×K	1001.84	Joback Method
cpg	1165.84	J/mol×K	969.08	Joback Method
cpg	1148.65	J/mol×K	936.31	Joback Method
cpg	1130.34	J/mol×K	903.55	Joback Method
cpg	1211.03	J/mol×K	1067.36	Joback Method
dvisc	0.0000077	Pa×s	870.79	Joback Method

dvisc	0.0000120	Pa×s	801.61	Joback Method
dvisc	0.0000205	Pa×s	732.42	Joback Method
dvisc	0.0000389	Pa×s	663.23	Joback Method
dvisc	0.0000858	Pa×s	594.05	Joback Method
dvisc	0.0002333	Pa×s	524.87	Joback Method
dvisc	0.0008594	Pa×s	455.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414310&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