Ethyl 3-hydroxydocosanoate

Inchi: InChI=1S/C24H48O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23(25)22-24
InchiKey: VJPPKNNPTLDPFE-UHFFFAOYSA-N
Formula: C24H48O3
SMILES: CCCCCCCCCCCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]: 384.64

Physical Properties

Property code	Value	Unit	Source
gf	-221.98	kJ/mol	Joback Method
hf	-941.00	kJ/mol	Joback Method
hfus	61.27	kJ/mol	Joback Method
hvap	94.46	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.342		Crippen Method
mcvol	362.330	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2749.90		NIST Webbook
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tb	916.55	K	Joback Method
tc	1128.69	K	Joback Method
tf	478.22	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1236.99	J/mol×K	916.55	Joback Method
cpg	1328.44	J/mol×K	1093.34	Joback Method
cpg	1312.71	J/mol×K	1057.98	Joback Method
cpg	1295.75	J/mol×K	1022.62	Joback Method
cpg	1277.52	J/mol×K	987.26	Joback Method
cpg	1257.96	J/mol×K	951.91	Joback Method
cpg	1343.01	J/mol×K	1128.69	Joback Method
dvisc	0.0000053	Pa×s	916.55	Joback Method

dvisc	0.0000082	Pa×s	843.50	Joback Method
dvisc	0.0000140	Pa×s	770.44	Joback Method
dvisc	0.0000265	Pa×s	697.38	Joback Method
dvisc	0.0000582	Pa×s	624.33	Joback Method
dvisc	0.0001576	Pa×s	551.27	Joback Method
dvisc	0.0005791	Pa×s	478.22	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=U414311&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume