

Ethyl 3-hydroxytetracosanoate

Inchi:	InChI=1S/C26H52O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25(27
InchiKey:	WMKVMTYMEYVFEN-UHFFFAOYSA-N
Formula:	C26H52O3
SMILES:	CCCCCCCCCCCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]:	412.69
CAS:	57402-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-205.14	kJ/mol	Joback Method
hf	-982.28	kJ/mol	Joback Method
hfus	66.45	kJ/mol	Joback Method
hvap	98.92	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.122		Crippen Method
mcvol	390.510	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	2956.60		NIST Webbook
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tb	962.31	K	Joback Method
tc	1194.82	K	Joback Method
tf	500.76	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.33	J/molxK	962.31	Joback Method
cpg	1388.02	J/molxK	1001.06	Joback Method
cpg	1409.02	J/molxK	1039.81	Joback Method
cpg	1428.41	J/molxK	1078.57	Joback Method
cpg	1446.29	J/molxK	1117.32	Joback Method
cpg	1462.73	J/molxK	1156.07	Joback Method
cpg	1477.82	J/molxK	1194.82	Joback Method

dvisc	0.0003907	Paxs	500.76	Joback Method
dvisc	0.0001066	Paxs	577.68	Joback Method
dvisc	0.0000395	Paxs	654.61	Joback Method
dvisc	0.0000180	Paxs	731.53	Joback Method
dvisc	0.0000095	Paxs	808.46	Joback Method
dvisc	0.0000056	Paxs	885.38	Joback Method
dvisc	0.0000036	Paxs	962.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57402376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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