(9Z,12Z,15Z)-1-Hydroxy-3-methoxypropan-2-yl octadeca-9,12,15-trienoate

Inchi: InChI=1S/C22H38O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22(24)26-21(19-23)2

InchiKey: FQKUVMVFEWKKLJ-YSTUJMKBSA-N

Formula: C22H38O4

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OC(CO)COC

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-103.16	kJ/mol	Joback Method
hf	-680.28	kJ/mol	Joback Method
hfus	57.88	kJ/mol	Joback Method
hvap	92.30	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.126		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2663.80		NIST Webbook
rinpol	2663.80		NIST Webbook
tb	905.69	K	Joback Method
tc	1109.01	K	Joback Method
tf	462.67	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.39	J/mol×K	905.69	Joback Method
cpg	1078.91	J/mol×K	939.58	Joback Method
cpg	1095.47	J/mol×K	973.46	Joback Method
cpg	1111.14	J/mol×K	1007.35	Joback Method
cpg	1125.98	J/mol×K	1041.24	Joback Method
cpg	1140.05	J/mol×K	1075.13	Joback Method
cpg	1153.43	J/mol×K	1109.01	Joback Method
dvisc	0.0004459	Pa×s	462.67	Joback Method

dvisc	0.0001149	Pa×s	536.51	Joback Method
dvisc	0.0000411	Pa×s	610.34	Joback Method
dvisc	0.0000184	Pa×s	684.18	Joback Method
dvisc	0.0000096	Pa×s	758.02	Joback Method
dvisc	0.0000056	Pa×s	831.85	Joback Method
dvisc	0.0000036	Pa×s	905.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412847&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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