

(6Z,9Z,12Z)-1-Hydroxy-3-methoxypropan-2-yl octadeca-6,9,12-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:	WXJXHVVWFHVIRRU-JPFHKJGASA-N
Formula:	C22H38O4
SMILES:	CCCCC=CCC=CC=CCCCC(=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	2634.80		NIST Webbook
rinpol	2634.80		NIST Webbook
tb	905.69	K	Joback Method
tc	1109.01	K	Joback Method
tf	462.67	K	Joback Method
vc	1.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001149	Paxs	536.51	Joback Method
dvisc	0.0000411	Paxs	610.34	Joback Method
dvisc	0.0000184	Paxs	684.18	Joback Method
dvisc	0.0000096	Paxs	758.02	Joback Method
dvisc	0.0000056	Paxs	831.85	Joback Method
dvisc	0.0000036	Paxs	905.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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