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

Inchi: InChI=1S/C22H40O4/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: NZORTWJTPAPCMO-NQLNTKRDSA-N

Formula: C22H40O4

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

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-183.38	kJ/mol	Joback Method
hf	-797.50	kJ/mol	Joback Method
hfus	57.68	kJ/mol	Joback Method
hvap	92.34	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.350		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	1042.60	kPa	Joback Method
rinpol	2654.60		NIST Webbook
rinpol	2654.60		NIST Webbook
tb	901.53	K	Joback Method
tc	1104.50	K	Joback Method
tf	467.75	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.70	J/mol×K	901.53	Joback Method
cpg	1106.78	J/mol×K	935.36	Joback Method
cpg	1123.79	J/mol×K	969.19	Joback Method
cpg	1139.78	J/mol×K	1003.02	Joback Method
cpg	1154.80	J/mol×K	1036.85	Joback Method
cpg	1168.90	J/mol×K	1070.68	Joback Method
cpg	1182.14	J/mol×K	1104.50	Joback Method
dvisc	0.0004619	Pa×s	467.75	Joback Method

dvisc	0.0001245	Pa×s	540.05	Joback Method
dvisc	0.0000457	Pa×s	612.34	Joback Method
dvisc	0.0000207	Pa×s	684.64	Joback Method
dvisc	0.0000109	Pa×s	756.94	Joback Method
dvisc	0.0000065	Pa×s	829.23	Joback Method
dvisc	0.0000041	Pa×s	901.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412848&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

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