1-Hydroxy-3-methoxypropan-2-yl oleate

Inchi: InChI=1S/C22H42O4/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: YNKCMMABCCJEQO-KHPPLWFESA-N
Formula: C22H42O4
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OC(CO)COC
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-263.60	kJ/mol	Joback Method
hf	-914.72	kJ/mol	Joback Method
hfus	57.48	kJ/mol	Joback Method
hvap	92.38	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.574		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	1008.45	kPa	Joback Method
rinpol	2656.20		NIST Webbook
rinpol	2656.20		NIST Webbook
tb	897.37	K	Joback Method
tc	1100.38	K	Joback Method
tf	472.83	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.86	J/mol×K	897.37	Joback Method
cpg	1134.57	J/mol×K	931.20	Joback Method
cpg	1152.09	J/mol×K	965.04	Joback Method
cpg	1168.45	J/mol×K	998.87	Joback Method
cpg	1183.70	J/mol×K	1032.71	Joback Method
cpg	1197.89	J/mol×K	1066.54	Joback Method
cpg	1211.06	J/mol×K	1100.38	Joback Method
dvisc	0.0004791	Pa×s	472.83	Joback Method

dvisc	0.0001348	Pa×s	543.59	Joback Method
dvisc	0.0000508	Pa×s	614.34	Joback Method
dvisc	0.0000234	Pa×s	685.10	Joback Method
dvisc	0.0000125	Pa×s	755.86	Joback Method
dvisc	0.0000074	Pa×s	826.61	Joback Method
dvisc	0.0000048	Pa×s	897.37	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=U412812&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