(6Z,9Z,12Z)-1,3-Dimethoxypropan-2-yl octadeca-6,9,12-trienoate

Inchi: InChI=1S/C23H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)27-22(20-25
InchiKey: VIKUDDUNJKSMIM-ORZIMQNZSA-N
Formula: C23H40O4
SMILES: CCCCCC=CCC=CCC=CCCCCC(=O)OC(COC)COC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-62.92	kJ/mol	Joback Method
hf	-680.91	kJ/mol	Joback Method
hfus	57.57	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.781		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	2578.80		NIST Webbook
rinpol	2578.80		NIST Webbook
tb	858.81	K	Joback Method
tc	1052.68	K	Joback Method
tf	435.35	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1083.66	J/mol×K	858.81	Joback Method
cpg	1102.70	J/mol×K	891.12	Joback Method
cpg	1120.66	J/mol×K	923.43	Joback Method
cpg	1137.61	J/mol×K	955.74	Joback Method
cpg	1153.57	J/mol×K	988.06	Joback Method
cpg	1168.60	J/mol×K	1020.37	Joback Method
cpg	1182.75	J/mol×K	1052.68	Joback Method
dvisc	0.0005205	Pa×s	435.35	Joback Method

dvisc	0.0001956	Pa×s	505.93	Joback Method
dvisc	0.0000934	Pa×s	576.50	Joback Method
dvisc	0.0000524	Pa×s	647.08	Joback Method
dvisc	0.0000329	Pa×s	717.66	Joback Method
dvisc	0.0000225	Pa×s	788.23	Joback Method
dvisc	0.0000164	Pa×s	858.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412796&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