

(9Z,12Z,15Z)-2,3-Dimethoxypropyl octadeca-9,12,15-trienoate

Inchi:	InChI=1S/C23H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)27-21-22(26)
InchiKey:	BCNRPQLYGMNZFE-AGRJPVHOSA-N
Formula:	C23H40O4
SMILES:	CCC=CCC=CCC=CCCCCCCC(=O)OCC(COC)OC
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
mvol	341.210	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	2571.80		NIST Webbook
rinpol	2571.80		NIST Webbook
tb	858.81	K	Joback Method
tc	1052.68	K	Joback Method
tf	435.35	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001956	Paxs	505.93	Joback Method
dvisc	0.0000934	Paxs	576.50	Joback Method
dvisc	0.0000524	Paxs	647.08	Joback Method
dvisc	0.0000329	Paxs	717.66	Joback Method
dvisc	0.0000225	Paxs	788.23	Joback Method
dvisc	0.0000164	Paxs	858.81	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412850&Units=SI

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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