

(9Z,12Z)-2,3-Dimethoxypropyl octadeca-9,12-dienoate

Inchi:	InChI=1S/C23H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)27-21-22(26)
InchiKey:	HVNUDBVUNSBEN-MURFETPASA-N
Formula:	C23H42O4
SMILES:	CCCCC=CCC=CCCCCCCCC(=O)OCC(COC)OC
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-143.14	kJ/mol	Joback Method
hf	-798.13	kJ/mol	Joback Method
hfus	57.37	kJ/mol	Joback Method
hvap	80.30	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.005		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2563.10		NIST Webbook
rinpol	2563.10		NIST Webbook
tb	854.65	K	Joback Method
tc	1046.80	K	Joback Method
tf	440.43	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.83	J/molxK	854.65	Joback Method
cpg	1129.43	J/molxK	886.68	Joback Method
cpg	1147.88	J/molxK	918.70	Joback Method
cpg	1165.22	J/molxK	950.73	Joback Method
cpg	1181.49	J/molxK	982.75	Joback Method
cpg	1196.71	J/molxK	1014.78	Joback Method
cpg	1210.94	J/molxK	1046.80	Joback Method
dvisc	0.0005551	Paxs	440.43	Joback Method

dvisc	0.0002153	Paxs	509.47	Joback Method
dvisc	0.0001046	Paxs	578.50	Joback Method
dvisc	0.0000593	Paxs	647.54	Joback Method
dvisc	0.0000375	Paxs	716.58	Joback Method
dvisc	0.0000257	Paxs	785.61	Joback Method
dvisc	0.0000187	Paxs	854.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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