

(Z)-1,3-Dimethoxypropan-2-yl octadec-11-enoate

Inchi:	InChI=1S/C23H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)27-22(20-25)
InchiKey:	DLLNKWFNKXPOHQ-KTKRTIGZSA-N
Formula:	C23H44O4
SMILES:	CCCCCCC=CCCCCCCCCCC(=O)OC(COC)COC
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-223.36	kJ/mol	Joback Method
hf	-915.35	kJ/mol	Joback Method
hfus	57.17	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.229		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	850.49	K	Joback Method
tc	1041.30	K	Joback Method
tf	445.51	K	Joback Method
vc	1.357	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1135.83	J/molxK	850.49	Joback Method
cpg	1156.03	J/molxK	882.29	Joback Method
cpg	1175.01	J/molxK	914.09	Joback Method
cpg	1192.80	J/molxK	945.90	Joback Method
cpg	1209.42	J/molxK	977.70	Joback Method
cpg	1224.90	J/molxK	1009.50	Joback Method
cpg	1239.27	J/molxK	1041.30	Joback Method
dvisc	0.0005923	Paxs	445.51	Joback Method

dvisc	0.0002369	Paxs	513.01	Joback Method
dvisc	0.0001173	Paxs	580.50	Joback Method
dvisc	0.0000672	Paxs	648.00	Joback Method
dvisc	0.0000428	Paxs	715.50	Joback Method
dvisc	0.0000294	Paxs	782.99	Joback Method
dvisc	0.0000215	Paxs	850.49	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412795&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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