(Z)-1,3-Dimethoxypropan-2-yl docos-13-enoate

Inchi: InChI=1S/C27H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-27(28
InchiKey: BYVHUGYWFIJQMS-QXMHVHEDSA-N
Formula: C27H52O4
SMILES: CCCCCCCCC=CCCCCCCCCCCCC(=O)OC(COC)COC
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-189.68	kJ/mol	Joback Method
hf	-997.91	kJ/mol	Joback Method
hfus	67.53	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.789		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	3008.70		NIST Webbook
tb	942.01	K	Joback Method
tc	1159.93	K	Joback Method
tf	490.59	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.71	J/mol×K	942.01	Joback Method
cpg	1414.17	J/mol×K	978.33	Joback Method
cpg	1434.94	J/mol×K	1014.65	Joback Method
cpg	1454.06	J/mol×K	1050.97	Joback Method
cpg	1471.60	J/mol×K	1087.29	Joback Method
cpg	1487.60	J/mol×K	1123.61	Joback Method
cpg	1502.12	J/mol×K	1159.93	Joback Method
dvisc	0.0003479	Pa×s	490.59	Joback Method
dvisc	0.0001355	Pa×s	565.83	Joback Method

dvisc	0.0000658	Pa×s	641.06	Joback Method
dvisc	0.0000372	Pa×s	716.30	Joback Method
dvisc	0.0000235	Pa×s	791.54	Joback Method
dvisc	0.0000160	Pa×s	866.77	Joback Method
dvisc	0.0000116	Pa×s	942.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412822&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