1,3-Dimethoxypropan-2-yl oleate

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: MXNZEXVRYIHIKT-QXMHVHEDSA-N
Formula: C23H44O4
SMILES: CCCCCCCCC=CCCCCCCCC(=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
mcvol	349.810	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2603.40		NIST Webbook
rinpol	2603.40		NIST Webbook
tb	850.49	K	Joback Method
tc	1041.30	K	Joback Method
tf	445.51	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002369	Pa×s	513.01	Joback Method
dvisc	0.0001173	Pa×s	580.50	Joback Method
dvisc	0.0000672	Pa×s	648.00	Joback Method
dvisc	0.0000428	Pa×s	715.50	Joback Method
dvisc	0.0000294	Pa×s	782.99	Joback Method
dvisc	0.0000215	Pa×s	850.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412846&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

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