1,3-Dimethoxypropan-2-yl stearate

Inchi: InChI=1S/C23H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)27-22(20-25
InchiKey: LEBHYYRSLSCGAZ-UHFFFAOYSA-N
Formula: C23H46O4
SMILES: CCCCCCCCCCCCCCCCCC(=O)OC(COC)COC
Mol. weight [g/mol]: 386.61

Physical Properties

Property code	Value	Unit	Source
gf	-303.58	kJ/mol	Joback Method
hf	-1032.57	kJ/mol	Joback Method
hfus	56.97	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.452		Crippen Method
mcvol	354.110	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2624.80		NIST Webbook
rinpol	2624.80		NIST Webbook
tb	846.33	K	Joback Method
tc	1036.17	K	Joback Method
tf	450.59	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.64	J/mol×K	846.33	Joback Method
cpg	1182.50	J/mol×K	877.97	Joback Method
cpg	1202.06	J/mol×K	909.61	Joback Method
cpg	1220.35	J/mol×K	941.25	Joback Method
cpg	1237.38	J/mol×K	972.89	Joback Method
cpg	1253.16	J/mol×K	1004.53	Joback Method
cpg	1267.73	J/mol×K	1036.17	Joback Method
dvisc	0.0006323	Pa×s	450.59	Joback Method

dvisc	0.0002607	Pa×s	516.55	Joback Method
dvisc	0.0001314	Pa×s	582.50	Joback Method
dvisc	0.0000761	Pa×s	648.46	Joback Method
dvisc	0.0000488	Pa×s	714.42	Joback Method
dvisc	0.0000337	Pa×s	780.37	Joback Method
dvisc	0.0000247	Pa×s	846.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412852&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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