3-(Octadecyloxy)propyl oleate

Inchi: InChI=1S/C39H76O3/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-36-41-37-34-38-
InchiKey: DGJSXVYZCNEXGC-ZZEZOPTASA-N
Formula: C39H76O3
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCCCOCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 593.02

Physical Properties

Property code	Value	Unit	Source
gf	18.80	kJ/mol	Joback Method
hf	-1108.09	kJ/mol	Joback Method
hfus	100.94	kJ/mol	Joback Method
hvap	113.93	kJ/mol	Joback Method
log10ws	-13.95		Crippen Method
logp	13.235		Crippen Method
mcvol	569.380	ml/mol	McGowan Method
pc	419.74	kPa	Joback Method
rinpol	402.80		NIST Webbook
rinpol	403.60		NIST Webbook
rinpol	385.30		NIST Webbook
tb	1194.59	K	Joback Method
tc	1624.89	K	Joback Method
tf	618.60	K	Joback Method
vc	2.241	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2162.48	J/mol×K	1194.59	Joback Method
cpg	2200.64	J/mol×K	1266.31	Joback Method
cpg	2233.75	J/mol×K	1338.02	Joback Method
cpg	2262.65	J/mol×K	1409.74	Joback Method
cpg	2288.19	J/mol×K	1481.46	Joback Method
cpg	2311.22	J/mol×K	1553.17	Joback Method
cpg	2332.57	J/mol×K	1624.89	Joback Method

dvisc	0.0000799	Pa×s	618.60	Joback Method
dvisc	0.0000304	Pa×s	714.60	Joback Method
dvisc	0.0000146	Pa×s	810.60	Joback Method
dvisc	0.0000081	Pa×s	906.59	Joback Method
dvisc	0.0000051	Pa×s	1002.59	Joback Method
dvisc	0.0000035	Pa×s	1098.59	Joback Method
dvisc	0.0000025	Pa×s	1194.59	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=R516566&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