1-(Nonanoyloxy)-3-(octanoyloxy)propan-2-yl decanoate

Inchi: InChI=1S/C30H56O6/c1-4-7-10-13-15-18-21-24-30(33)36-27(25-34-28(31)22-19-16-12-9

InchiKey: PKMKZQZKAMXXQN-UHFFFAOYSA-N

Formula: C30H56O6

SMILES: CCCCCCCCCC(=O)OC(COC(=O)CCCCCCC)COC(=O)CCCCCCCCC

Mol. weight [g/mol]: 512.76

Physical Properties

Property code	Value	Unit	Source
gf	-502.48	kJ/mol	Joback Method
hf	-1402.21	kJ/mol	Joback Method
hfus	78.29	kJ/mol	Joback Method
hvap	109.45	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	8.236		Crippen Method
mcvol	455.880	ml/mol	McGowan Method
pc	640.27	kPa	Joback Method
rinpol	3221.50		NIST Webbook
rinpol	3221.50		NIST Webbook
tb	1114.23	K	Joback Method
tc	1417.46	K	Joback Method
tf	629.34	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1649.32	J/mol×K	1114.23	Joback Method
cpg	1716.52	J/mol×K	1366.92	Joback Method
cpg	1709.60	J/mol×K	1316.38	Joback Method
cpg	1699.54	J/mol×K	1265.84	Joback Method
cpg	1686.22	J/mol×K	1215.31	Joback Method
cpg	1669.52	J/mol×K	1164.77	Joback Method
cpg	1720.41	J/mol×K	1417.46	Joback Method
dvisc	0.0000069	Pa×s	1114.23	Joback Method

dvisc	0.0000094	Pa×s	1033.41	Joback Method
dvisc	0.0000133	Pa×s	952.60	Joback Method
dvisc	0.0000202	Pa×s	871.78	Joback Method
dvisc	0.0000333	Pa×s	790.97	Joback Method
dvisc	0.0000617	Pa×s	710.15	Joback Method
dvisc	0.0001337	Pa×s	629.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413787&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