2-(Nonanoyloxy)propane-1,3-diyl dioctanoate

Inchi: InChI=1S/C28H52O6/c1-4-7-10-13-16-19-22-28(31)34-25(23-32-26(29)20-17-14-11-8-5-
InchiKey: PVGJWYNUBYUGJV-UHFFFAOYSA-N
Formula: C28H52O6
SMILES: CCCCCCCCC(=O)OC(COC(=O)CCCCCCC)COC(=O)CCCCCCC
Mol. weight [g/mol]: 484.71

Physical Properties

Property code	Value	Unit	Source
gf	-519.32	kJ/mol	Joback Method
hf	-1360.93	kJ/mol	Joback Method
hfus	73.11	kJ/mol	Joback Method
hvap	105.00	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.456		Crippen Method
mcvol	427.700	ml/mol	McGowan Method
pc	707.33	kPa	Joback Method
rinpol	3042.60		NIST Webbook
rinpol	3042.60		NIST Webbook
tb	1068.47	K	Joback Method
tc	1339.10	K	Joback Method
tf	606.80	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.90	J/mol×K	1068.47	Joback Method
cpg	1592.11	J/mol×K	1294.00	Joback Method
cpg	1583.31	J/mol×K	1248.89	Joback Method
cpg	1571.96	J/mol×K	1203.79	Joback Method
cpg	1557.99	J/mol×K	1158.68	Joback Method
cpg	1541.33	J/mol×K	1113.58	Joback Method
cpg	1598.43	J/mol×K	1339.10	Joback Method
dvisc	0.0000097	Pa×s	1068.47	Joback Method

dvisc	0.0000130	Pa×s	991.52	Joback Method
dvisc	0.0000184	Pa×s	914.58	Joback Method
dvisc	0.0000277	Pa×s	837.63	Joback Method
dvisc	0.0000454	Pa×s	760.69	Joback Method
dvisc	0.0000832	Pa×s	683.75	Joback Method
dvisc	0.0001776	Pa×s	606.80	Joback Method

Sources

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=U412804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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