2-(Decanoyloxy)-3-(octanoyloxy)propyl benzoate

Inchi: InChI=1S/C28H44O6/c1-3-5-7-9-10-12-17-21-27(30)34-25(22-32-26(29)20-16-11-8-6-4-2
InchiKey: UHMVKVMCXUDQLN-UHFFFAOYSA-N
Formula: C28H44O6
SMILES: CCCCCCCCCC(=O)OC(COC(=O)CCCCCCC)COC(=O)c1ccccc1
Mol. weight [g/mol]: 476.65

Physical Properties

Property code	Value	Unit	Source
gf	-406.91	kJ/mol	Joback Method
hf	-1124.40	kJ/mol	Joback Method
hfus	67.16	kJ/mol	Joback Method
hvap	107.28	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.800		Crippen Method
mcvol	403.940	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	3207.50		NIST Webbook
rinpol	3207.50		NIST Webbook
tb	1095.15	K	Joback Method
tc	1352.51	K	Joback Method
tf	633.22	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.47	J/mol×K	1095.15	Joback Method
cpg	1461.08	J/mol×K	1309.62	Joback Method
cpg	1454.98	J/mol×K	1266.72	Joback Method
cpg	1446.84	J/mol×K	1223.83	Joback Method
cpg	1436.60	J/mol×K	1180.94	Joback Method
cpg	1424.16	J/mol×K	1138.04	Joback Method
cpg	1465.21	J/mol×K	1352.51	Joback Method
dvisc	0.0000100	Pa×s	1095.15	Joback Method

dvisc	0.0000133	Pa×s	1018.16	Joback Method
dvisc	0.0000185	Pa×s	941.17	Joback Method
dvisc	0.0000274	Pa×s	864.19	Joback Method
dvisc	0.0000437	Pa×s	787.20	Joback Method
dvisc	0.0000771	Pa×s	710.21	Joback Method
dvisc	0.0001561	Pa×s	633.22	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=U413788&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