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

Inchi: InChI=1S/C29H54O6/c1-4-7-10-13-14-17-20-23-29(32)35-26(24-33-27(30)21-18-15-11-8
InchiKey: GVUCZFUFLQMFID-UHFFFAOYSA-N
Formula: C29H54O6
SMILES: CCCCCCCCCC(=O)OC(COC(=O)CCCCCCC)COC(=O)CCCCCCC
Mol. weight [g/mol]: 498.74
CAS: 33368-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-510.90	kJ/mol	Joback Method
hf	-1381.57	kJ/mol	Joback Method
hfus	75.70	kJ/mol	Joback Method
hvap	107.23	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.846		Crippen Method
mcvol	441.790	ml/mol	McGowan Method
pc	672.55	kPa	Joback Method
rinpol	3137.50		NIST Webbook
rinpol	3137.50		NIST Webbook
tb	1091.35	K	Joback Method
tc	1377.37	K	Joback Method
tf	618.07	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.55	J/mol×K	1091.35	Joback Method
cpg	1605.37	J/mol×K	1139.02	Joback Method
cpg	1622.08	J/mol×K	1186.69	Joback Method
cpg	1635.78	J/mol×K	1234.36	Joback Method
cpg	1646.56	J/mol×K	1282.03	Joback Method
cpg	1654.52	J/mol×K	1329.70	Joback Method
cpg	1659.73	J/mol×K	1377.37	Joback Method

dvisc	0.0001543	Pa×s	618.07	Joback Method
dvisc	0.0000717	Pa×s	696.95	Joback Method
dvisc	0.0000389	Pa×s	775.83	Joback Method
dvisc	0.0000237	Pa×s	854.71	Joback Method
dvisc	0.0000157	Pa×s	933.59	Joback Method
dvisc	0.0000110	Pa×s	1012.47	Joback Method
dvisc	0.0000082	Pa×s	1091.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33368875&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

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