3-(Octanoyloxy)propane-1,2-diyl bis(decanoate)

Inchi: InChI=1S/C31H58O6/c1-4-7-10-13-15-18-21-24-30(33)36-27-28(26-35-29(32)23-20-17-1
InchiKey: KHOXIGZKRZJQTF-UHFFFAOYSA-N
Formula: C31H58O6
SMILES: CCCCCCCCCC(=O)OCC(COC(=O)CCCCCCC)OC(=O)CCCCCCCCC
Mol. weight [g/mol]: 526.79
CAS: 82426-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-494.06	kJ/mol	Joback Method
hf	-1422.85	kJ/mol	Joback Method
hfus	80.88	kJ/mol	Joback Method
hvap	111.68	kJ/mol	Joback Method
log10ws	-9.50		Crippen Method
logp	8.627		Crippen Method
mcvol	469.970	ml/mol	McGowan Method
pc	610.27	kPa	Joback Method
rinpol	3348.10		NIST Webbook
rinpol	3348.10		NIST Webbook
tb	1137.11	K	Joback Method
tc	1459.53	K	Joback Method
tf	640.61	K	Joback Method
vc	1.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1713.18	J/mol×K	1137.11	Joback Method
cpg	1733.74	J/mol×K	1190.85	Joback Method
cpg	1750.34	J/mol×K	1244.58	Joback Method
cpg	1763.15	J/mol×K	1298.32	Joback Method
cpg	1772.30	J/mol×K	1352.06	Joback Method
cpg	1777.97	J/mol×K	1405.79	Joback Method
cpg	1780.30	J/mol×K	1459.53	Joback Method

dvisc	0.0001157	Pa×s	640.61	Joback Method
dvisc	0.0000530	Pa×s	723.36	Joback Method
dvisc	0.0000285	Pa×s	806.11	Joback Method
dvisc	0.0000172	Pa×s	888.86	Joback Method
dvisc	0.0000113	Pa×s	971.61	Joback Method
dvisc	0.0000079	Pa×s	1054.36	Joback Method
dvisc	0.0000059	Pa×s	1137.11	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=C82426888&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