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

Inchi: InChI=1S/C26H48O6/c1-4-7-10-13-16-18-24(27)30-21-23(32-26(29)20-15-12-9-6-3)22-3
InchiKey: DGYZDFDBZWEASX-UHFFFAOYSA-N
Formula: C26H48O6
SMILES: CCCCCCCC(=O)OCC(COC(=O)CCCCCCC)OC(=O)CCCCCC
Mol. weight [g/mol]: 456.66
CAS: 1204770-16-0

Physical Properties

Property code	Value	Unit	Source
gf	-536.16	kJ/mol	Joback Method
hf	-1319.65	kJ/mol	Joback Method
hfus	67.93	kJ/mol	Joback Method
hvap	100.55	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.676		Crippen Method
mcvol	399.520	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	2842.70		NIST Webbook
rinpol	2842.70		NIST Webbook
tb	1022.71	K	Joback Method
tc	1267.51	K	Joback Method
tf	584.26	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.14	J/mol×K	1022.71	Joback Method
cpg	1413.78	J/mol×K	1063.51	Joback Method
cpg	1430.19	J/mol×K	1104.31	Joback Method
cpg	1444.44	J/mol×K	1145.11	Joback Method
cpg	1456.56	J/mol×K	1185.91	Joback Method
cpg	1466.58	J/mol×K	1226.71	Joback Method
cpg	1474.57	J/mol×K	1267.51	Joback Method

dvisc	0.0002341	Pa×s	584.26	Joback Method
dvisc	0.0001114	Pa×s	657.34	Joback Method
dvisc	0.0000615	Pa×s	730.41	Joback Method
dvisc	0.0000379	Pa×s	803.49	Joback Method
dvisc	0.0000253	Pa×s	876.56	Joback Method
dvisc	0.0000179	Pa×s	949.63	Joback Method
dvisc	0.0000134	Pa×s	1022.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1204770160&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