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

Inchi: InChI=1S/C26H40O6/c1-3-5-7-9-14-18-24(27)30-20-23(32-25(28)19-15-10-8-6-4-2)21-31
InchiKey: CAVVDWNDQLBBCW-UHFFFAOYSA-N
Formula: C26H40O6
SMILES: CCCCCCCC(=O)OCC(COC(=O)c1ccccc1)OC(=O)CCCCCCC
Mol. weight [g/mol]: 448.59

Physical Properties

Property code	Value	Unit	Source
gf	-423.75	kJ/mol	Joback Method
hf	-1083.12	kJ/mol	Joback Method
hfus	61.98	kJ/mol	Joback Method
hvap	102.83	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.019		Crippen Method
mcvol	375.760	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	3016.40		NIST Webbook
rinpol	3016.40		NIST Webbook
tb	1049.39	K	Joback Method
tc	1288.14	K	Joback Method
tf	610.68	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.97	J/mol×K	1049.39	Joback Method
cpg	1300.44	J/mol×K	1089.18	Joback Method
cpg	1312.99	J/mol×K	1128.97	Joback Method
cpg	1323.67	J/mol×K	1168.77	Joback Method
cpg	1332.53	J/mol×K	1208.56	Joback Method
cpg	1339.63	J/mol×K	1248.35	Joback Method
cpg	1345.01	J/mol×K	1288.14	Joback Method
dvisc	0.0002043	Pa×s	610.68	Joback Method

dvisc	0.0001026	Pa×s	683.80	Joback Method
dvisc	0.0000588	Pa×s	756.92	Joback Method
dvisc	0.0000372	Pa×s	830.03	Joback Method
dvisc	0.0000254	Pa×s	903.15	Joback Method
dvisc	0.0000183	Pa×s	976.27	Joback Method
dvisc	0.0000138	Pa×s	1049.39	Joback Method

Sources

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=U413809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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