Terephthalic acid, 2-chloropropyl hexadecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-31-26(29)24-17-19-25

InchiKey: OJPGGBHGOSPFPB-UHFFFAOYSA-N

Formula: C27H43ClO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1

Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-202.97	kJ/mol	Joback Method
hf	-886.17	kJ/mol	Joback Method
hfus	65.59	kJ/mol	Joback Method
hvap	100.94	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.109		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpol	3400.00		NIST Webbook
rinpol	3400.00		NIST Webbook
tb	1038.39	K	Joback Method
tc	1274.58	K	Joback Method
tf	592.23	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.45	J/mol×K	1038.39	Joback Method
cpg	1349.03	J/mol×K	1077.76	Joback Method
cpg	1363.88	J/mol×K	1117.12	Joback Method
cpg	1377.09	J/mol×K	1156.49	Joback Method
cpg	1388.73	J/mol×K	1195.85	Joback Method
cpg	1398.85	J/mol×K	1235.22	Joback Method
cpg	1407.54	J/mol×K	1274.58	Joback Method
dvisc	0.0002302	Pa×s	592.23	Joback Method

dvisc	0.0001129	Pa×s	666.59	Joback Method
dvisc	0.0000639	Pa×s	740.95	Joback Method
dvisc	0.0000401	Pa×s	815.31	Joback Method
dvisc	0.0000272	Pa×s	889.67	Joback Method
dvisc	0.0000196	Pa×s	964.03	Joback Method
dvisc	0.0000148	Pa×s	1038.39	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=U356181&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