Terephthalic acid, 2-chloropropyl heptadecyl ester

Inchi: InChI=1S/C28H45ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-32-27(30)25-18-20

InchiKey: HLPYNBDEQKURGT-UHFFFAOYSA-N

Formula: C28H45ClO4

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

Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-194.55	kJ/mol	Joback Method
hf	-906.81	kJ/mol	Joback Method
hfus	68.18	kJ/mol	Joback Method
hvap	103.17	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.499		Crippen Method
mcvol	408.740	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	3503.00		NIST Webbook
tb	1061.27	K	Joback Method
tc	1306.03	K	Joback Method
tf	603.50	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.16	J/mol×K	1061.27	Joback Method
cpg	1412.04	J/mol×K	1102.06	Joback Method
cpg	1427.07	J/mol×K	1142.86	Joback Method
cpg	1440.34	J/mol×K	1183.65	Joback Method
cpg	1451.92	J/mol×K	1224.44	Joback Method
cpg	1461.91	J/mol×K	1265.23	Joback Method
cpg	1470.38	J/mol×K	1306.03	Joback Method
dvisc	0.0002016	Pa×s	603.50	Joback Method
dvisc	0.0000981	Pa×s	679.79	Joback Method

dvisc	0.0000552	Pa×s	756.09	Joback Method
dvisc	0.0000345	Pa×s	832.38	Joback Method
dvisc	0.0000233	Pa×s	908.68	Joback Method
dvisc	0.0000168	Pa×s	984.98	Joback Method
dvisc	0.0000126	Pa×s	1061.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356182&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