Phthalic acid, 2-(3-chlorophenyl)ethyl tetradecyl ester

Inchi: InChI=1S/C30H41ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-15-22-34-29(32)27-19-13-14-20-28(

InchiKey: DAPQZYUCVZACJQ-UHFFFAOYSA-N

Formula: C30H41ClO4

SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1

Mol. weight [g/mol]: 501.10

Physical Properties

Property code	Value	Unit	Source
gf	-72.49	kJ/mol	Joback Method
hf	-717.75	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	110.95	kJ/mol	Joback Method
log10ws	-10.12		Crippen Method
logp	8.597		Crippen Method
mcvol	413.160	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	3712.00		NIST Webbook
rinpol	3712.00		NIST Webbook
tb	1139.13	K	Joback Method
tc	1400.38	K	Joback Method
tf	679.98	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.35	J/mol×K	1139.13	Joback Method
cpg	1417.94	J/mol×K	1182.67	Joback Method
cpg	1429.68	J/mol×K	1226.21	Joback Method
cpg	1439.68	J/mol×K	1269.76	Joback Method
cpg	1448.07	J/mol×K	1313.30	Joback Method
cpg	1454.94	J/mol×K	1356.84	Joback Method
cpg	1460.42	J/mol×K	1400.38	Joback Method
dvisc	0.0001174	Pa×s	679.98	Joback Method

dvisc	0.0000647	Pa×s	756.50	Joback Method
dvisc	0.0000398	Pa×s	833.03	Joback Method
dvisc	0.0000265	Pa×s	909.56	Joback Method
dvisc	0.0000188	Pa×s	986.08	Joback Method
dvisc	0.0000141	Pa×s	1062.61	Joback Method
dvisc	0.0000109	Pa×s	1139.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377864&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