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

Inchi: InChI=1S/C29H39ClO4/c1-2-3-4-5-6-7-8-9-10-11-14-21-33-28(31)26-18-12-13-19-27(26)
InchiKey: KREOLZKJAOMQSD-UHFFFAOYSA-N
Formula: C29H39ClO4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 487.07

Physical Properties

Property code	Value	Unit	Source
gf	-80.91	kJ/mol	Joback Method
hf	-697.11	kJ/mol	Joback Method
hfus	67.94	kJ/mol	Joback Method
hvap	108.72	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	8.207		Crippen Method
mcvol	399.070	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	3610.00		NIST Webbook
tb	1116.25	K	Joback Method
tc	1369.17	K	Joback Method
tf	668.71	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1342.53	J/mol×K	1116.25	Joback Method
cpg	1355.96	J/mol×K	1158.40	Joback Method
cpg	1367.65	J/mol×K	1200.56	Joback Method
cpg	1377.69	J/mol×K	1242.71	Joback Method
cpg	1386.18	J/mol×K	1284.86	Joback Method
cpg	1393.22	J/mol×K	1327.01	Joback Method
cpg	1398.90	J/mol×K	1369.17	Joback Method
dvisc	0.0001336	Pa×s	668.71	Joback Method
dvisc	0.0000743	Pa×s	743.30	Joback Method

dvisc	0.0000459	Pa×s	817.89	Joback Method
dvisc	0.0000308	Pa×s	892.48	Joback Method
dvisc	0.0000220	Pa×s	967.07	Joback Method
dvisc	0.0000164	Pa×s	1041.66	Joback Method
dvisc	0.0000128	Pa×s	1116.25	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U377863&Units=SI

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