Phthalic acid, 4-chloro-2-methylphenyl tetradecyl ester

Inchi: InChI=1S/C29H39ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-16-21-33-28(31)25-17-14-15-18-26

InchiKey: JXIUUQBIIMUKJG-UHFFFAOYSA-N

Formula: C29H39ClO4

SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 487.07

Physical Properties

Property code	Value	Unit	Source
gf	-90.54	kJ/mol	Joback Method
hf	-708.58	kJ/mol	Joback Method
hfus	67.55	kJ/mol	Joback Method
hvap	109.38	kJ/mol	Joback Method
log10ws	-10.40		Crippen Method
logp	8.726		Crippen Method
mcvol	399.070	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpol	3558.00		NIST Webbook
rinpol	3558.00		NIST Webbook
tb	1121.23	K	Joback Method
tc	1375.45	K	Joback Method
tf	681.23	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.00	J/mol×K	1121.23	Joback Method
cpg	1354.13	J/mol×K	1163.60	Joback Method
cpg	1365.43	J/mol×K	1205.97	Joback Method
cpg	1374.99	J/mol×K	1248.34	Joback Method
cpg	1382.91	J/mol×K	1290.71	Joback Method
cpg	1389.27	J/mol×K	1333.08	Joback Method
cpg	1394.16	J/mol×K	1375.45	Joback Method
dvisc	0.0001223	Pa×s	681.23	Joback Method

dvisc	0.0000705	Pa×s	754.56	Joback Method
dvisc	0.0000448	Pa×s	827.90	Joback Method
dvisc	0.0000306	Pa×s	901.23	Joback Method
dvisc	0.0000222	Pa×s	974.56	Joback Method
dvisc	0.0000168	Pa×s	1047.90	Joback Method
dvisc	0.0000132	Pa×s	1121.23	Joback Method

Sources

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=U356380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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