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

Inchi: InChI=1S/C28H37ClO4/c1-2-3-4-5-6-7-8-9-10-13-20-32-27(30)25-17-11-12-18-26(25)28(

InchiKey: ZZHRZGJDOMXEBB-UHFFFAOYSA-N

Formula: C28H37ClO4

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

Mol. weight [g/mol]: 473.04

Physical Properties

Property code	Value	Unit	Source
gf	-89.33	kJ/mol	Joback Method
hf	-676.47	kJ/mol	Joback Method
hfus	65.35	kJ/mol	Joback Method
hvap	106.50	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	7.817		Crippen Method
mcvol	384.980	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	3509.00		NIST Webbook
rinpol	3509.00		NIST Webbook
tb	1093.37	K	Joback Method
tc	1339.26	K	Joback Method
tf	657.44	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.99	J/mol×K	1093.37	Joback Method
cpg	1294.29	J/mol×K	1134.35	Joback Method
cpg	1305.94	J/mol×K	1175.33	Joback Method
cpg	1316.02	J/mol×K	1216.32	Joback Method
cpg	1324.61	J/mol×K	1257.30	Joback Method
cpg	1331.80	J/mol×K	1298.28	Joback Method
cpg	1337.67	J/mol×K	1339.26	Joback Method
dvisc	0.0001517	Pa×s	657.44	Joback Method

dvisc	0.0000851	Pa×s	730.10	Joback Method
dvisc	0.0000530	Pa×s	802.75	Joback Method
dvisc	0.0000357	Pa×s	875.40	Joback Method
dvisc	0.0000256	Pa×s	948.06	Joback Method
dvisc	0.0000192	Pa×s	1020.71	Joback Method
dvisc	0.0000150	Pa×s	1093.37	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=U377862&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