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

Inchi: InChI=1S/C24H29ClO4/c1-2-3-4-5-6-9-16-28-23(26)21-13-7-8-14-22(21)24(27)29-17-15-
InchiKey: YZICJXOKOMPLMI-UHFFFAOYSA-N
Formula: C24H29ClO4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 416.94

Physical Properties

Property code	Value	Unit	Source
gf	-123.01	kJ/mol	Joback Method
hf	-593.91	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	97.59	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.257		Crippen Method
mcvol	328.620	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	3107.00		NIST Webbook
tb	1001.85	K	Joback Method
tc	1231.17	K	Joback Method
tf	612.36	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.35	J/mol×K	1001.85	Joback Method
cpg	1051.32	J/mol×K	1040.07	Joback Method
cpg	1062.88	J/mol×K	1078.29	Joback Method
cpg	1073.08	J/mol×K	1116.51	Joback Method
cpg	1081.98	J/mol×K	1154.73	Joback Method
cpg	1089.64	J/mol×K	1192.95	Joback Method
cpg	1096.10	J/mol×K	1231.17	Joback Method
dvisc	0.0002457	Pa×s	612.36	Joback Method
dvisc	0.0001434	Pa×s	677.27	Joback Method

dvisc	0.0000919	Pa×s	742.19	Joback Method
dvisc	0.0000633	Pa×s	807.11	Joback Method
dvisc	0.0000461	Pa×s	872.02	Joback Method
dvisc	0.0000350	Pa×s	936.93	Joback Method
dvisc	0.0000276	Pa×s	1001.85	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=U377858&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