Phthalic acid, 2-(4-chlorophenoxy)ethyl octyl ester

Inchi: InChI=1S/C24H29ClO5/c1-2-3-4-5-6-11-16-29-23(26)19-12-7-8-13-20(19)24(27)30-18-17

InchiKey: HKESLZLWLPTJTC-UHFFFAOYSA-N

Formula: C24H29ClO5

SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 432.94

Physical Properties

Property code	Value	Unit	Source
gf	-228.01	kJ/mol	Joback Method
hf	-726.13	kJ/mol	Joback Method
hfus	56.18	kJ/mol	Joback Method
hvap	100.00	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.093		Crippen Method
mcvol	334.490	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	3179.00		NIST Webbook
rinpol	3179.00		NIST Webbook
tb	1024.27	K	Joback Method
tc	1256.29	K	Joback Method
tf	634.59	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.46	J/mol×K	1024.27	Joback Method
cpg	1076.32	J/mol×K	1062.94	Joback Method
cpg	1086.58	J/mol×K	1101.61	Joback Method
cpg	1095.28	J/mol×K	1140.28	Joback Method
cpg	1102.45	J/mol×K	1178.95	Joback Method
cpg	1108.13	J/mol×K	1217.62	Joback Method
cpg	1112.35	J/mol×K	1256.29	Joback Method
dvisc	0.0001726	Pa×s	634.59	Joback Method

dvisc	0.0001025	Pa×s	699.54	Joback Method
dvisc	0.0000665	Pa×s	764.48	Joback Method
dvisc	0.0000461	Pa×s	829.43	Joback Method
dvisc	0.0000338	Pa×s	894.38	Joback Method
dvisc	0.0000258	Pa×s	959.32	Joback Method
dvisc	0.0000204	Pa×s	1024.27	Joback Method

Sources

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=U377909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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