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

Inchi: InChI=1S/C22H25ClO5/c1-2-3-4-9-14-27-21(24)17-10-5-6-11-18(17)22(25)28-16-15-26-2

InchiKey: YQEUOPSLRZXRLY-UHFFFAOYSA-N

Formula: C22H25ClO5

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

Mol. weight [g/mol]: 404.88

Physical Properties

Property code	Value	Unit	Source
gf	-244.85	kJ/mol	Joback Method
hf	-684.85	kJ/mol	Joback Method
hfus	51.00	kJ/mol	Joback Method
hvap	95.55	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.313		Crippen Method
mcvol	306.310	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	978.51	K	Joback Method
tc	1206.59	K	Joback Method
tf	612.05	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.09	J/mol×K	978.51	Joback Method
cpg	958.00	J/mol×K	1016.52	Joback Method
cpg	968.42	J/mol×K	1054.54	Joback Method
cpg	977.39	J/mol×K	1092.55	Joback Method
cpg	984.92	J/mol×K	1130.57	Joback Method
cpg	991.06	J/mol×K	1168.58	Joback Method
cpg	995.81	J/mol×K	1206.59	Joback Method
dvisc	0.0002173	Pa×s	612.05	Joback Method

dvisc	0.0001317	Pa×s	673.13	Joback Method
dvisc	0.0000868	Pa×s	734.20	Joback Method
dvisc	0.0000610	Pa×s	795.28	Joback Method
dvisc	0.0000450	Pa×s	856.36	Joback Method
dvisc	0.0000346	Pa×s	917.43	Joback Method
dvisc	0.0000275	Pa×s	978.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377907&Units=SI
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

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