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

Inchi: InChI=1S/C21H23ClO5/c1-2-3-8-13-26-20(23)16-9-4-5-10-17(16)21(24)27-15-14-25-19-1

InchiKey: ZXQVFFOMYMKEDL-UHFFFAOYSA-N

Formula: C21H23ClO5

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

Mol. weight [g/mol]: 390.86

Physical Properties

Property code	Value	Unit	Source
gf	-253.27	kJ/mol	Joback Method
hf	-664.21	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	93.32	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.923		Crippen Method
mcvol	292.220	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2880.00		NIST Webbook
tb	955.63	K	Joback Method
tc	1183.11	K	Joback Method
tf	600.78	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.62	J/mol×K	955.63	Joback Method
cpg	933.04	J/mol×K	1145.20	Joback Method
cpg	926.74	J/mol×K	1107.29	Joback Method
cpg	919.07	J/mol×K	1069.37	Joback Method
cpg	910.01	J/mol×K	1031.46	Joback Method
cpg	899.53	J/mol×K	993.54	Joback Method
cpg	937.99	J/mol×K	1183.11	Joback Method
dvisc	0.0000319	Pa×s	955.63	Joback Method
dvisc	0.0000400	Pa×s	896.49	Joback Method

dvisc	0.0000519	Pa×s	837.35	Joback Method
dvisc	0.0000699	Pa×s	778.21	Joback Method
dvisc	0.0000988	Pa×s	719.06	Joback Method
dvisc	0.0001488	Pa×s	659.92	Joback Method
dvisc	0.0002427	Pa×s	600.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377906&Units=SI

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

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