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

Inchi: InChI=1S/C23H27ClO5/c1-2-3-4-5-10-15-28-22(25)18-11-6-7-12-19(18)23(26)29-17-16-2

InchiKey: ZIRLTJWGQJBHFE-UHFFFAOYSA-N

Formula: C23H27ClO5

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

Mol. weight [g/mol]: 418.91

Physical Properties

Property code	Value	Unit	Source
gf	-236.43	kJ/mol	Joback Method
hf	-705.49	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	97.78	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.703		Crippen Method
mcvol	320.400	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	3082.00		NIST Webbook
rinpol	3082.00		NIST Webbook
tb	1001.39	K	Joback Method
tc	1230.96	K	Joback Method
tf	623.32	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.06	J/mol×K	1001.39	Joback Method
cpg	1016.94	J/mol×K	1039.65	Joback Method
cpg	1027.29	J/mol×K	1077.91	Joback Method
cpg	1036.14	J/mol×K	1116.18	Joback Method
cpg	1043.51	J/mol×K	1154.44	Joback Method
cpg	1049.44	J/mol×K	1192.70	Joback Method
cpg	1053.95	J/mol×K	1230.96	Joback Method
dvisc	0.0001940	Pa×s	623.32	Joback Method

dvisc	0.0001164	Pa×s	686.33	Joback Method
dvisc	0.0000761	Pa×s	749.34	Joback Method
dvisc	0.0000531	Pa×s	812.36	Joback Method
dvisc	0.0000390	Pa×s	875.37	Joback Method
dvisc	0.0000299	Pa×s	938.38	Joback Method
dvisc	0.0000237	Pa×s	1001.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377908&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