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

Inchi: InChI=1S/C20H21ClO5/c1-14(2)13-26-20(23)16-8-4-3-7-15(16)19(22)25-12-11-24-18-10

InchiKey: AUXZBRRFVVUULA-UHFFFAOYSA-N

Formula: C20H21ClO5

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 376.83

Physical Properties

Property code	Value	Unit	Source
gf	-264.13	kJ/mol	Joback Method
hf	-648.85	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.389		Crippen Method
mcvol	278.130	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	932.31	K	Joback Method
tc	1162.42	K	Joback Method
tf	574.51	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.21	J/mol×K	932.31	Joback Method
cpg	875.87	J/mol×K	1124.07	Joback Method
cpg	869.54	J/mol×K	1085.72	Joback Method
cpg	861.82	J/mol×K	1047.36	Joback Method
cpg	852.71	J/mol×K	1009.01	Joback Method
cpg	842.18	J/mol×K	970.66	Joback Method
cpg	880.84	J/mol×K	1162.42	Joback Method
dvisc	0.0000337	Pa×s	932.31	Joback Method

dvisc	0.0000427	Pa×s	872.68	Joback Method
dvisc	0.0000560	Pa×s	813.04	Joback Method
dvisc	0.0000766	Pa×s	753.41	Joback Method
dvisc	0.0001107	Pa×s	693.78	Joback Method
dvisc	0.0001714	Pa×s	634.14	Joback Method
dvisc	0.0002906	Pa×s	574.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377904&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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