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

Inchi: InChI=1S/C20H21ClO5/c1-2-3-12-25-19(22)15-8-4-5-9-16(15)20(23)26-14-13-24-18-11-7

InchiKey: RYLKTLAWYMWOQE-UHFFFAOYSA-N

Formula: C20H21ClO5

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

Mol. weight [g/mol]: 376.83

Physical Properties

Property code	Value	Unit	Source
gf	-261.69	kJ/mol	Joback Method
hf	-643.57	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	91.10	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.533		Crippen Method
mcvol	278.130	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2781.00		NIST Webbook
rinpol	2781.00		NIST Webbook
tb	932.75	K	Joback Method
tc	1160.48	K	Joback Method
tf	589.51	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.70	J/mol×K	932.75	Joback Method
cpg	875.42	J/mol×K	1122.52	Joback Method
cpg	868.99	J/mol×K	1084.57	Joback Method
cpg	861.22	J/mol×K	1046.61	Joback Method
cpg	852.10	J/mol×K	1008.66	Joback Method
cpg	841.60	J/mol×K	970.70	Joback Method
cpg	880.52	J/mol×K	1160.48	Joback Method
dvisc	0.0000369	Pa×s	932.75	Joback Method

dvisc	0.0000462	Pa×s	875.54	Joback Method
dvisc	0.0000596	Pa×s	818.34	Joback Method
dvisc	0.0000798	Pa×s	761.13	Joback Method
dvisc	0.0001122	Pa×s	703.92	Joback Method
dvisc	0.0001675	Pa×s	646.72	Joback Method
dvisc	0.0002702	Pa×s	589.51	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=U377905&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