Benzoic acid, 2-(2-chlorophenoxy)ethyl ester

Inchi: InChI=1S/C15H13ClO3/c16-13-8-4-5-9-14(13)18-10-11-19-15(17)12-6-2-1-3-7-12/h1-9H
InchiKey: WEVUWIBFSSKMIB-UHFFFAOYSA-N
Formula: C15H13ClO3
SMILES: O=C(OCCOc1ccccc1Cl)c1ccccc1
Mol. weight [g/mol]: 276.71

Physical Properties

Property code	Value	Unit	Source
gf	-60.24	kJ/mol	Joback Method
hf	-284.10	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	70.15	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.576		Crippen Method
mcvol	200.240	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	737.08	K	Joback Method
tc	974.54	K	Joback Method
tf	448.48	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.53	J/mol×K	737.08	Joback Method
cpg	530.35	J/mol×K	776.66	Joback Method
cpg	543.00	J/mol×K	816.23	Joback Method
cpg	554.52	J/mol×K	855.81	Joback Method
cpg	564.94	J/mol×K	895.38	Joback Method
cpg	574.28	J/mol×K	934.96	Joback Method
cpg	582.59	J/mol×K	974.54	Joback Method
dvisc	0.0007901	Pa×s	448.48	Joback Method

dvisc	0.0004705	Pa×s	496.58	Joback Method
dvisc	0.0003070	Pa×s	544.68	Joback Method
dvisc	0.0002147	Pa×s	592.78	Joback Method
dvisc	0.0001585	Pa×s	640.88	Joback Method
dvisc	0.0001220	Pa×s	688.98	Joback Method
dvisc	0.0000972	Pa×s	737.08	Joback Method

Sources

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=U368259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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