Phthalic acid, 2-(4-chlorophenyl)ethyl ethyl ester

Inchi: InChI=1S/C18H17ClO4/c1-2-22-17(20)15-5-3-4-6-16(15)18(21)23-12-11-13-7-9-14(19)1

InchiKey: WFLFKQLNMQIRKN-UHFFFAOYSA-N

Formula: C18H17ClO4

SMILES: CCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 332.78

Physical Properties

Property code	Value	Unit	Source
gf	-173.53	kJ/mol	Joback Method
hf	-470.07	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.916		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	864.57	K	Joback Method
tc	1096.73	K	Joback Method
tf	544.74	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.86	J/mol×K	864.57	Joback Method
cpg	702.33	J/mol×K	903.26	Joback Method
cpg	713.55	J/mol×K	941.96	Joback Method
cpg	723.58	J/mol×K	980.65	Joback Method
cpg	732.42	J/mol×K	1019.35	Joback Method
cpg	740.12	J/mol×K	1058.04	Joback Method
cpg	746.70	J/mol×K	1096.73	Joback Method
dvisc	0.0004610	Pa×s	544.74	Joback Method

dvisc	0.0002879	Pa×s	598.04	Joback Method
dvisc	0.0001942	Pa×s	651.35	Joback Method
dvisc	0.0001390	Pa×s	704.65	Joback Method
dvisc	0.0001043	Pa×s	757.96	Joback Method
dvisc	0.0000813	Pa×s	811.26	Joback Method
dvisc	0.0000653	Pa×s	864.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377835&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

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