

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

Inchi:	InChI=1S/C18H17ClO5/c1-2-22-17(20)13-7-3-4-8-14(13)18(21)24-12-11-23-16-10-6-5-9
InchiKey:	JNZMOAUMCLVTTI-UHFFFAOYSA-N
Formula:	C18H17ClO5
SMILES:	CCOC(=O)c1cccc1C(=O)OCCOc1cccc1Cl
Mol. weight [g/mol]:	348.78

Physical Properties

Property code	Value	Unit	Source
gf	-278.53	kJ/mol	Joback Method
hf	-602.29	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.752		Crippen Method
mcvol	249.950	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	886.99	K	Joback Method
tc	1117.53	K	Joback Method
tf	566.97	K	Joback Method
vc	0.943	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.76	J/molxK	886.99	Joback Method
cpg	761.53	J/molxK	1079.11	Joback Method
cpg	754.98	J/molxK	1040.69	Joback Method
cpg	747.15	J/molxK	1002.26	Joback Method
cpg	738.00	J/molxK	963.84	Joback Method
cpg	727.55	J/molxK	925.41	Joback Method
cpg	766.80	J/molxK	1117.53	Joback Method
dvisc	0.0000491	Paxs	886.99	Joback Method

dvisc	0.0000610	Paxs	833.65	Joback Method
dvisc	0.0000779	Paxs	780.32	Joback Method
dvisc	0.0001033	Paxs	726.98	Joback Method
dvisc	0.0001433	Paxs	673.64	Joback Method
dvisc	0.0002101	Paxs	620.31	Joback Method
dvisc	0.0003311	Paxs	566.97	Joback Method

Sources

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=U377902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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