

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

Inchi:	InChI=1S/C24H20Cl2O6/c25-19-9-3-5-11-21(19)29-13-15-31-23(27)17-7-1-2-8-18(17)24
InchiKey:	HQFYPHPERZCZGU-UHFFFAOYSA-N
Formula:	C24H20Cl2O6
SMILES:	O=C(OCCOc1cccc1Cl)c1cccc1C(=O)OCCOc1cccc1Cl
Mol. weight [g/mol]:	475.32

Physical Properties

Property code	Value	Unit	Source
gf	-242.16	kJ/mol	Joback Method
hf	-649.03	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	109.73	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.465		Crippen Method
mcvol	328.840	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	3623.00		NIST Webbook
tb	1115.78	K	Joback Method
tc	1371.78	K	Joback Method
tf	725.68	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.98	J/molxK	1115.78	Joback Method
cpg	991.35	J/molxK	1158.45	Joback Method
cpg	994.76	J/molxK	1201.11	Joback Method
cpg	996.24	J/molxK	1243.78	Joback Method
cpg	995.83	J/molxK	1286.44	Joback Method
cpg	993.55	J/molxK	1329.11	Joback Method
cpg	989.42	J/molxK	1371.78	Joback Method
dvisc	0.0000856	Paxs	725.68	Joback Method
dvisc	0.0000554	Paxs	790.70	Joback Method

dvisc	0.0000383	Paxs	855.71	Joback Method
dvisc	0.0000279	Paxs	920.73	Joback Method
dvisc	0.0000212	Paxs	985.75	Joback Method
dvisc	0.0000166	Paxs	1050.76	Joback Method
dvisc	0.0000135	Paxs	1115.78	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=U377916&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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