

# Isophthalic acid, 4-chlorophenyl pentyl ester

<b>Inchi:</b>	InChI=1S/C19H19ClO4/c1-2-3-4-12-23-18(21)14-6-5-7-15(13-14)19(22)24-17-10-8-16(20)
<b>InchiKey:</b>	AHJWJYOJIOEACF-UHFFFAOYSA-N
<b>Formula:</b>	C19H19ClO4
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
<b>Mol. weight [g/mol]:</b>	346.81

## Physical Properties

Property code	Value	Unit	Source
gf	-165.11	kJ/mol	Joback Method
hf	-490.71	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.906		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinsol	2782.00		NIST Webbook
tb	887.45	K	Joback Method
tc	1117.22	K	Joback Method
tf	556.01	K	Joback Method
vc	0.981	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.25	J/molxK	887.45	Joback Method
cpg	758.85	J/molxK	925.75	Joback Method
cpg	770.20	J/molxK	964.04	Joback Method
cpg	780.32	J/molxK	1002.34	Joback Method
cpg	789.24	J/molxK	1040.63	Joback Method
cpg	797.01	J/molxK	1078.93	Joback Method
cpg	803.66	J/molxK	1117.22	Joback Method
dvisc	0.0004190	Paxs	556.01	Joback Method
dvisc	0.0002585	Paxs	611.25	Joback Method

dvisc	0.0001728	Paxs	666.49	Joback Method
dvisc	0.0001228	Paxs	721.73	Joback Method
dvisc	0.0000917	Paxs	776.97	Joback Method
dvisc	0.0000711	Paxs	832.21	Joback Method
dvisc	0.0000569	Paxs	887.45	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344579&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344579&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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