

# Isophthalic acid, 6-chlorohexyl pentyl ester

<b>Inchi:</b>	InChI=1S/C19H27ClO4/c1-2-3-7-13-23-18(21)16-10-9-11-17(15-16)19(22)24-14-8-5-4-6
<b>InchiKey:</b>	ALALRFOFOBOCJF-UHFFFAOYSA-N
<b>Formula:</b>	C19H27ClO4
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)OCCCCC(Cl)c1
<b>Mol. weight [g/mol]:</b>	354.87

## Physical Properties

Property code	Value	Unit	Source
gf	-267.89	kJ/mol	Joback Method
hf	-715.77	kJ/mol	Joback Method
hfus	48.39	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.990		Crippen Method
mvol	281.930	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	855.79	K	Joback Method
tc	1060.17	K	Joback Method
tf	517.07	K	Joback Method
vc	1.089	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.29	J/molxK	855.79	Joback Method
cpg	909.23	J/molxK	1026.10	Joback Method
cpg	898.76	J/molxK	992.04	Joback Method
cpg	887.26	J/molxK	957.98	Joback Method
cpg	874.69	J/molxK	923.92	Joback Method
cpg	861.04	J/molxK	889.85	Joback Method
cpg	918.69	J/molxK	1060.17	Joback Method
dvisc	0.0000546	Paxs	855.79	Joback Method

dvisc	0.0000698	Paxs	799.34	Joback Method
dvisc	0.0000928	Paxs	742.88	Joback Method
dvisc	0.0001292	Paxs	686.43	Joback Method
dvisc	0.0001909	Paxs	629.98	Joback Method
dvisc	0.0003045	Paxs	573.52	Joback Method
dvisc	0.0005380	Paxs	517.07	Joback Method

## Sources

<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=U345880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345880&amp;Units=SI</a>
<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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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