

# Isophthalic acid, 2,4-dichlorophenyl hexyl ester

Inchi:	InChI=1S/C20H20Cl2O4/c1-2-3-4-5-11-25-19(23)14-7-6-8-15(12-14)20(24)26-18-10-9-16
InchiKey:	LGKZMUXZOSFZKR-UHFFFAOYSA-N
Formula:	C20H20Cl2O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	395.28

## Physical Properties

Property code	Value	Unit	Source
gf	-178.25	kJ/mol	Joback Method
hf	-538.56	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.950		Crippen Method
mvol	284.500	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		NIST Webbook
tb	952.74	K	Joback Method
tc	1185.41	K	Joback Method
tf	609.72	K	Joback Method
vc	1.085	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.06	J/molxK	952.74	Joback Method
cpg	834.27	J/molxK	991.52	Joback Method
cpg	844.20	J/molxK	1030.30	Joback Method
cpg	852.87	J/molxK	1069.08	Joback Method
cpg	860.32	J/molxK	1107.86	Joback Method
cpg	866.57	J/molxK	1146.64	Joback Method
cpg	871.66	J/molxK	1185.41	Joback Method
dvisc	0.0002844	Paxs	609.72	Joback Method

dvisc	0.0001817	Paxs	666.89	Joback Method
dvisc	0.0001246	Paxs	724.06	Joback Method
dvisc	0.0000903	Paxs	781.23	Joback Method
dvisc	0.0000684	Paxs	838.40	Joback Method
dvisc	0.0000537	Paxs	895.57	Joback Method
dvisc	0.0000433	Paxs	952.74	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=U344410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344410&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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