

# Isophthalic acid, 2,5-dichlorophenyl propyl ester

Inchi:	InChI=1S/C17H14Cl2O4/c1-2-8-22-16(20)11-4-3-5-12(9-11)17(21)23-15-10-13(18)6-7-14
InchiKey:	ZLJOVBVIBNJLFZ-UHFFFAOYSA-N
Formula:	C17H14Cl2O4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1
Mol. weight [g/mol]:	353.20

## Physical Properties

Property code	Value	Unit	Source
gf	-203.51	kJ/mol	Joback Method
hf	-476.64	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.779		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	884.10	K	Joback Method
tc	1122.62	K	Joback Method
tf	575.91	K	Joback Method
vc	0.917	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.59	J/molxK	884.10	Joback Method
cpg	695.80	J/molxK	1082.87	Joback Method
cpg	689.70	J/molxK	1043.11	Joback Method
cpg	682.45	J/molxK	1003.36	Joback Method
cpg	674.03	J/molxK	963.61	Joback Method
cpg	664.42	J/molxK	923.85	Joback Method
cpg	700.78	J/molxK	1122.62	Joback Method
dvisc	0.0000663	Paxs	884.10	Joback Method

dvisc	0.0000811	Paxs	832.73	Joback Method
dvisc	0.0001020	Paxs	781.37	Joback Method
dvisc	0.0001325	Paxs	730.00	Joback Method
dvisc	0.0001791	Paxs	678.64	Joback Method
dvisc	0.0002542	Paxs	627.28	Joback Method
dvisc	0.0003841	Paxs	575.91	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=U344697&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344697&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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