

# Isophthalic acid, 2,6-dichlorophenyl octyl ester

Inchi:	InChI=1S/C22H24Cl2O4/c1-2-3-4-5-6-7-14-27-21(25)16-10-8-11-17(15-16)22(26)28-20-
InchiKey:	PGMDQFVTNYOMLJ-UHFFFAOYSA-N
Formula:	C22H24Cl2O4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1
Mol. weight [g/mol]:	423.33

## Physical Properties

Property code	Value	Unit	Source
gf	-161.41	kJ/mol	Joback Method
hf	-579.84	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	98.19	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.730		Crippen Method
mvol	312.680	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	3172.00		NIST Webbook
rinpol	3172.00		NIST Webbook
tb	998.50	K	Joback Method
tc	1231.29	K	Joback Method
tf	632.26	K	Joback Method
vc	1.198	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.27	J/molxK	998.50	Joback Method
cpg	982.86	J/molxK	1192.49	Joback Method
cpg	976.70	J/molxK	1153.69	Joback Method
cpg	969.29	J/molxK	1114.89	Joback Method
cpg	960.62	J/molxK	1076.10	Joback Method
cpg	950.62	J/molxK	1037.30	Joback Method
cpg	987.84	J/molxK	1231.29	Joback Method
dvisc	0.0000323	Paxs	998.50	Joback Method

dvisc	0.0000402	Paxs	937.46	Joback Method
dvisc	0.0000517	Paxs	876.42	Joback Method
dvisc	0.0000690	Paxs	815.38	Joback Method
dvisc	0.0000964	Paxs	754.34	Joback Method
dvisc	0.0001430	Paxs	693.30	Joback Method
dvisc	0.0002287	Paxs	632.26	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=U344626&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344626&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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