

# Isophthalic acid, 2,5-dichlorophenyl heptyl ester

Inchi:	InChI=1S/C21H22Cl2O4/c1-2-3-4-5-6-12-26-20(24)15-8-7-9-16(13-15)21(25)27-19-14-17
InchiKey:	DHQFMYIBOMXKFN-UHFFFAOYSA-N
Formula:	C21H22Cl2O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1
Mol. weight [g/mol]:	409.30

## Physical Properties

Property code	Value	Unit	Source
gf	-169.83	kJ/mol	Joback Method
hf	-559.20	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	95.96	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.340		Crippen Method
mvol	298.590	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	3114.00		NIST Webbook
rinpol	3114.00		NIST Webbook
tb	975.62	K	Joback Method
tc	1207.92	K	Joback Method
tf	620.99	K	Joback Method
vc	1.141	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.88	J/molxK	975.62	Joback Method
cpg	924.49	J/molxK	1169.20	Joback Method
cpg	918.26	J/molxK	1130.49	Joback Method
cpg	910.83	J/molxK	1091.77	Joback Method
cpg	902.14	J/molxK	1053.05	Joback Method
cpg	892.17	J/molxK	1014.34	Joback Method
cpg	929.54	J/molxK	1207.92	Joback Method
dvisc	0.0000375	Paxs	975.62	Joback Method

dvisc	0.0000465	Paxs	916.51	Joback Method
dvisc	0.0000595	Paxs	857.41	Joback Method
dvisc	0.0000790	Paxs	798.30	Joback Method
dvisc	0.0001098	Paxs	739.20	Joback Method
dvisc	0.0001614	Paxs	680.10	Joback Method
dvisc	0.0002554	Paxs	620.99	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344703&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344703&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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