

# Isophthalic acid, 8-chlorooctyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C22H33ClO4/c1-18(2)11-10-16-27-22(25)20-13-9-12-19(17-20)21(24)26-15-8
<b>InchiKey:</b>	ZHQFRDCEPFXFJT-UHFFFAOYSA-N
<b>Formula:</b>	C22H33ClO4
<b>SMILES:</b>	CC(C)CCCOC(=O)c1cccc(C(=O)OCCCCCCCCl)c1
<b>Mol. weight [g/mol]:</b>	396.95

## Physical Properties

Property code	Value	Unit	Source
gf	-245.07	kJ/mol	Joback Method
hf	-782.97	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	89.81	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.016		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	923.99	K	Joback Method
tc	1134.49	K	Joback Method
tf	535.88	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.82	J/molxK	923.99	Joback Method
cpg	1040.24	J/molxK	959.07	Joback Method
cpg	1054.38	J/molxK	994.16	Joback Method
cpg	1067.27	J/molxK	1029.24	Joback Method
cpg	1078.94	J/molxK	1064.32	Joback Method
cpg	1089.43	J/molxK	1099.41	Joback Method
cpg	1098.78	J/molxK	1134.49	Joback Method
dvisc	0.0004300	Paxs	535.88	Joback Method

dvisc	0.0002211	Paxs	600.57	Joback Method
dvisc	0.0001294	Paxs	665.25	Joback Method
dvisc	0.0000832	Paxs	729.93	Joback Method
dvisc	0.0000575	Paxs	794.62	Joback Method
dvisc	0.0000421	Paxs	859.30	Joback Method
dvisc	0.0000321	Paxs	923.99	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=U356389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356389&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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