

# Phthalic acid, di(8-chlorooctyl) ester

<b>Inchi:</b>	InChI=1S/C24H36Cl2O4/c25-17-11-5-1-3-7-13-19-29-23(27)21-15-9-10-16-22(21)24(28)
<b>InchiKey:</b>	YPCJGZCBPCZFGT-UHFFFAOYSA-N
<b>Formula:</b>	C24H36Cl2O4
<b>SMILES:</b>	O=C(OCCCCCCCCCl)c1ccccc1C(=O)OCCCCCCCCCl
<b>Mol. weight [g/mol]:</b>	459.45

## Physical Properties

Property code	Value	Unit	Source
gf	-237.72	kJ/mol	Joback Method
hf	-834.71	kJ/mol	Joback Method
hfus	65.54	kJ/mol	Joback Method
hvap	99.04	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.159		Crippen Method
mvol	364.620	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	1007.62	K	Joback Method
tc	1233.82	K	Joback Method
tf	603.34	K	Joback Method
vc	1.417	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.68	J/molxK	1007.62	Joback Method
cpg	1185.39	J/molxK	1045.32	Joback Method
cpg	1198.65	J/molxK	1083.02	Joback Method
cpg	1210.51	J/molxK	1120.72	Joback Method
cpg	1221.04	J/molxK	1158.42	Joback Method
cpg	1230.28	J/molxK	1196.12	Joback Method
cpg	1238.29	J/molxK	1233.82	Joback Method
dvisc	0.0002434	Paxs	603.34	Joback Method

dvisc	0.0001330	Paxs	670.72	Joback Method
dvisc	0.0000811	Paxs	738.10	Joback Method
dvisc	0.0000537	Paxs	805.48	Joback Method
dvisc	0.0000379	Paxs	872.86	Joback Method
dvisc	0.0000282	Paxs	940.24	Joback Method
dvisc	0.0000218	Paxs	1007.62	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=U356869&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356869&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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