

# Phthalic acid, 2,2-dichloroethyl octyl ester

<b>Inchi:</b>	InChI=1S/C18H24Cl2O4/c1-2-3-4-5-6-9-12-23-17(21)14-10-7-8-11-15(14)18(22)24-13-16
<b>InchiKey:</b>	DAXLVRXUCFHTRT-UHFFFAOYSA-N
<b>Formula:</b>	C18H24Cl2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc1C(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	375.29

## Physical Properties

Property code	Value	Unit	Source
gf	-290.68	kJ/mol	Joback Method
hf	-716.15	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.164		Crippen Method
mvol	280.080	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	869.90	K	Joback Method
tc	1080.66	K	Joback Method
tf	520.72	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.13	J/molxK	869.90	Joback Method
cpg	870.60	J/molxK	1045.54	Joback Method
cpg	861.43	J/molxK	1010.41	Joback Method
cpg	851.23	J/molxK	975.28	Joback Method
cpg	839.96	J/molxK	940.15	Joback Method
cpg	827.60	J/molxK	905.03	Joback Method
cpg	878.75	J/molxK	1080.66	Joback Method
dvisc	0.0000495	Paxs	869.90	Joback Method

dvisc	0.0000639	Paxs	811.70	Joback Method
dvisc	0.0000859	Paxs	753.51	Joback Method
dvisc	0.0001213	Paxs	695.31	Joback Method
dvisc	0.0001824	Paxs	637.11	Joback Method
dvisc	0.0002976	Paxs	578.92	Joback Method
dvisc	0.0005419	Paxs	520.72	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=U356929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356929&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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