

# Isophthalic acid, octyl phenylethyl ester

<b>Inchi:</b>	InChI=1S/C24H30O4/c1-2-3-4-5-6-10-17-27-23(25)21-14-11-15-22(19-21)24(26)28-18-1
<b>InchiKey:</b>	FZVHQJTUQGLRRX-UHFFFAOYSA-N
<b>Formula:</b>	C24H30O4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	382.49

## Physical Properties

Property code	Value	Unit	Source
gf	-101.45	kJ/mol	Joback Method
hf	-566.70	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.603		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	959.44	K	Joback Method
tc	1182.13	K	Joback Method
tf	569.92	K	Joback Method
vc	1.212	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.74	J/molxK	959.44	Joback Method
cpg	1031.19	J/molxK	996.55	Joback Method
cpg	1044.26	J/molxK	1033.67	Joback Method
cpg	1056.00	J/molxK	1070.78	Joback Method
cpg	1066.47	J/molxK	1107.90	Joback Method
cpg	1075.71	J/molxK	1145.01	Joback Method
cpg	1083.79	J/molxK	1182.13	Joback Method
dvisc	0.0003390	Paxs	569.92	Joback Method

dvisc	0.0001867	Paxs	634.84	Joback Method
dvisc	0.0001149	Paxs	699.76	Joback Method
dvisc	0.0000768	Paxs	764.68	Joback Method
dvisc	0.0000547	Paxs	829.60	Joback Method
dvisc	0.0000409	Paxs	894.52	Joback Method
dvisc	0.0000318	Paxs	959.44	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=U344339&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344339&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>

## 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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