

# Isophthalic acid, 2-methoxyethyl nonyl ester

<b>Inchi:</b>	InChI=1S/C20H30O5/c1-3-4-5-6-7-8-9-13-24-19(21)17-11-10-12-18(16-17)20(22)25-15-
<b>InchiKey:</b>	OOVAQRWXLBQXAM-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCOC)c1
<b>Mol. weight [g/mol]:</b>	350.45

## Physical Properties

Property code	Value	Unit	Source
gf	-352.54	kJ/mol	Joback Method
hf	-852.89	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	83.77	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.397		Crippen Method
mvol	289.650	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1065.19	K	Joback Method
tf	520.65	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.10	J/molxK	863.66	Joback Method
cpg	922.75	J/molxK	897.25	Joback Method
cpg	937.18	J/molxK	930.84	Joback Method
cpg	950.41	J/molxK	964.43	Joback Method
cpg	962.45	J/molxK	998.02	Joback Method
cpg	973.30	J/molxK	1031.61	Joback Method
cpg	982.99	J/molxK	1065.19	Joback Method
dvisc	0.0004161	Paxs	520.65	Joback Method

dvisc	0.0002338	Paxs	577.82	Joback Method
dvisc	0.0001457	Paxs	634.99	Joback Method
dvisc	0.0000982	Paxs	692.15	Joback Method
dvisc	0.0000703	Paxs	749.32	Joback Method
dvisc	0.0000527	Paxs	806.49	Joback Method
dvisc	0.0000411	Paxs	863.66	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=U345864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345864&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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