

# Isophthalic acid, isobutyl oct-3-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C20H28O4/c1-5-6-7-8-10-16(4)24-20(22)18-12-9-11-17(13-18)19(21)23-14-15
<b>InchiKey:</b>	DVEQFNVJVIDLMF-CSKARUKUSA-N
<b>Formula:</b>	C20H28O4
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	332.43

## Physical Properties

Property code	Value	Unit	Source
gf	-172.20	kJ/mol	Joback Method
hf	-614.01	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.791		Crippen Method
mvol	279.480	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	844.52	K	Joback Method
tc	1052.77	K	Joback Method
tf	463.34	K	Joback Method
vc	1.063	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.32	J/molxK	844.52	Joback Method
cpg	921.03	J/molxK	1018.06	Joback Method
cpg	909.42	J/molxK	983.35	Joback Method
cpg	896.78	J/molxK	948.64	Joback Method
cpg	883.08	J/molxK	913.94	Joback Method
cpg	868.27	J/molxK	879.23	Joback Method
cpg	931.64	J/molxK	1052.77	Joback Method
dvisc	0.0000401	Paxs	844.52	Joback Method

dvisc	0.0000534	Paxs	780.99	Joback Method
dvisc	0.0000747	Paxs	717.46	Joback Method
dvisc	0.0001116	Paxs	653.93	Joback Method
dvisc	0.0001818	Paxs	590.40	Joback Method
dvisc	0.0003330	Paxs	526.87	Joback Method
dvisc	0.0007202	Paxs	463.34	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=U343891&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343891&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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