

# Isophthalic acid, butyl 2-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C20H22O4/c1-3-5-13-23-19(21)16-10-8-11-17(14-16)20(22)24-18-12-7-6-9-15
<b>InchiKey:</b>	BZPHFPOOHQMAFR-UHFFFAOYSA-N
<b>Formula:</b>	C20H22O4
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CC)c1
<b>Mol. weight [g/mol]:</b>	326.39

## Physical Properties

Property code	Value	Unit	Source
gf	-144.76	kJ/mol	Joback Method
hf	-495.61	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.425		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	872.90	K	Joback Method
tc	1097.43	K	Joback Method
tf	537.36	K	Joback Method
vc	0.988	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.36	J/molxK	872.90	Joback Method
cpg	838.28	J/molxK	1060.01	Joback Method
cpg	829.14	J/molxK	1022.59	Joback Method
cpg	818.81	J/molxK	985.17	Joback Method
cpg	807.26	J/molxK	947.74	Joback Method
cpg	794.45	J/molxK	910.32	Joback Method
cpg	846.26	J/molxK	1097.43	Joback Method
dvisc	0.0000570	Paxs	872.90	Joback Method
dvisc	0.0000716	Paxs	816.98	Joback Method

dvisc	0.0000928	Paxs	761.05	Joback Method
dvisc	0.0001255	Paxs	705.13	Joback Method
dvisc	0.0001788	Paxs	649.21	Joback Method
dvisc	0.0002722	Paxs	593.28	Joback Method
dvisc	0.0004522	Paxs	537.36	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=U356762&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356762&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

Latest version available from:

<https://www.chemeo.com/cid/66-917-1/Isophthalic-acid-butyl-2-ethylphenyl-ester.pdf>

Generated by Cheméo on 2024-04-27 17:41:47.662443245 +0000 UTC m=+16528956.583020560.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.