

# Phthalic acid, butyl 3-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C20H22O5/c1-3-4-12-24-19(21)17-10-5-6-11-18(17)20(22)25-14-15-8-7-9-16(
<b>InchiKey:</b>	VYQBECNLWYYKAQ-UHFFFAOYSA-N
<b>Formula:</b>	C20H22O5
<b>SMILES:</b>	CCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC)c1
<b>Mol. weight [g/mol]:</b>	342.39

## Physical Properties

Property code	Value	Unit	Source
gf	-249.76	kJ/mol	Joback Method
hf	-627.83	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	86.71	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.009		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	2604.00		NIST Webbook
rinpol	2604.00		NIST Webbook
tb	895.32	K	Joback Method
tc	1119.10	K	Joback Method
tf	559.59	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.52	J/molxK	895.32	Joback Method
cpg	820.89	J/molxK	932.62	Joback Method
cpg	832.88	J/molxK	969.91	Joback Method
cpg	843.50	J/molxK	1007.21	Joback Method
cpg	852.78	J/molxK	1044.51	Joback Method
cpg	860.72	J/molxK	1081.80	Joback Method
cpg	867.35	J/molxK	1119.10	Joback Method
dvisc	0.0003238	Paxs	559.59	Joback Method

dvisc	0.0001984	Paxs	615.55	Joback Method
dvisc	0.0001319	Paxs	671.50	Joback Method
dvisc	0.0000933	Paxs	727.45	Joback Method
dvisc	0.0000694	Paxs	783.41	Joback Method
dvisc	0.0000537	Paxs	839.37	Joback Method
dvisc	0.0000429	Paxs	895.32	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377977&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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