

# Phthalic acid, butyl 3-methoxy-4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C20H21NO7/c1-3-4-11-27-19(22)15-7-5-6-8-16(15)20(23)28-13-14-9-10-17(21)
<b>InchiKey:</b>	BDKOOPIPMHRLHV-UHFFFAOYSA-N
<b>Formula:</b>	C20H21NO7
<b>SMILES:</b>	CCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
<b>Mol. weight [g/mol]:</b>	387.38

## Physical Properties

Property code	Value	Unit	Source
gf	-223.84	kJ/mol	Joback Method
hf	-650.06	kJ/mol	Joback Method
hfus	52.59	kJ/mol	Joback Method
hvap	103.97	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	3.917		Crippen Method
mvol	283.310	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	3484.00		NIST Webbook
rinpol	3484.00		NIST Webbook
tb	1052.14	K	Joback Method
tc	1298.21	K	Joback Method
tf	715.72	K	Joback Method
vc	1.087	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.73	J/mol×K	1052.14	Joback Method
cpg	906.00	J/mol×K	1093.15	Joback Method
cpg	912.60	J/mol×K	1134.16	Joback Method
cpg	917.52	J/mol×K	1175.18	Joback Method
cpg	920.79	J/mol×K	1216.19	Joback Method
cpg	922.43	J/mol×K	1257.20	Joback Method
cpg	922.45	J/mol×K	1298.21	Joback Method

# Sources

<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=U382532&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382532&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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