

# Phthalic acid, butyl 3,5-dinitro-4-methylbenzyl ester

Inchi:	InChI=1S/C20H20N2O8/c1-3-4-9-29-19(23)15-7-5-6-8-16(15)20(24)30-12-14-10-17(21)(2
InchiKey:	JUYUCYKRJYFWEQ-UHFFFAOYSA-N
Formula:	C20H20N2O8
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCc1cc([N+](=O)[O-])c(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	416.38

## Physical Properties

Property code	Value	Unit	Source
gf	-92.92	kJ/mol	Joback Method
hf	-540.07	kJ/mol	Joback Method
hfus	62.38	kJ/mol	Joback Method
hvap	118.81	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	4.125		Crippen Method
mvol	294.860	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook
tb	1186.54	K	Joback Method
tc	1456.55	K	Joback Method
tf	849.62	K	Joback Method
vc	1.151	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.92	J/molxK	1186.54	Joback Method
cpg	950.06	J/molxK	1231.54	Joback Method
cpg	952.49	J/molxK	1276.54	Joback Method
cpg	953.25	J/molxK	1321.54	Joback Method
cpg	952.39	J/molxK	1366.54	Joback Method
cpg	949.97	J/molxK	1411.55	Joback Method
cpg	946.04	J/molxK	1456.55	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=U415512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415512&amp;Units=SI</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>hvpap:</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>rinppl:</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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