

# Phthalic acid, 4-methyl-3-nitrobenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C24H29NO6/c1-3-4-5-6-7-10-15-30-23(26)20-11-8-9-12-21(20)24(27)31-17-19
<b>InchiKey:</b>	XGEYXGYSKQTLRS-UHFFFAOYSA-N
<b>Formula:</b>	C24H29NO6
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc1C(=O)OCc1ccc(C)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	427.49

## Physical Properties

Property code	Value	Unit	Source
gf	-85.16	kJ/mol	Joback Method
hf	-600.40	kJ/mol	Joback Method
hfus	61.77	kJ/mol	Joback Method
hvap	110.46	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	5.778		Crippen Method
mvol	333.800	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	3578.00		NIST Webbook
rinpol	3578.00		NIST Webbook
tb	1121.24	K	Joback Method
tc	1373.45	K	Joback Method
tf	738.57	K	Joback Method
vc	1.294	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.73	J/molxK	1121.24	Joback Method
cpg	1119.22	J/molxK	1163.27	Joback Method
cpg	1127.07	J/molxK	1205.31	Joback Method
cpg	1133.34	J/molxK	1247.34	Joback Method
cpg	1138.11	J/molxK	1289.38	Joback Method
cpg	1141.42	J/molxK	1331.41	Joback Method
cpg	1143.35	J/molxK	1373.45	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=U382586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382586&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>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>rinpola:</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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