

# Benzoic acid, (3-methoxy-4-nitrophenyl)methyl ester

Inchi:	InChI=1S/C15H13NO5/c1-20-14-9-11(7-8-13(14)16(18)19)10-21-15(17)12-5-3-2-4-6-12/
InchiKey:	BQFZSJMXRGHNMU-UHFFFAOYSA-N
Formula:	C15H13NO5
SMILES:	COc1cc(COC(=O)c2ccccc2)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	287.27

## Physical Properties

Property code	Value	Unit	Source
gf	-22.39	kJ/mol	Joback Method
hf	-290.59	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	2.960		Crippen Method
mcvol	205.420	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinqol	2536.00		NIST Webbook
tb	856.47	K	Joback Method
tc	1109.25	K	Joback Method
tf	574.69	K	Joback Method
vc	0.783	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.71	J/molxK	856.47	Joback Method
cpg	599.43	J/molxK	898.60	Joback Method
cpg	609.84	J/molxK	940.73	Joback Method
cpg	618.96	J/molxK	982.86	Joback Method
cpg	626.83	J/molxK	1024.99	Joback Method
cpg	633.48	J/molxK	1067.12	Joback Method
cpg	638.94	J/molxK	1109.25	Joback Method

# Sources

<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=U368931&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368931&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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