

# Benzoic acid, 4-nitroso-, methyl ester

**Inchi:** InChI=1S/C8H7NO3/c1-12-8(10)6-2-4-7(9-11)5-3-6/h2-5H,1H3  
**InchiKey:** CAFWWZWJFFJXTF-UHFFFAOYSA-N  
**Formula:** C8H7NO3  
**SMILES:** COC(=O)c1ccc(N=O)cc1  
**Mol. weight [g/mol]:** 165.15  
**CAS:** 13170-28-0

## Physical Properties

Property code	Value	Unit	Source
hf	-396.38	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.871		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	553.79	K	Joback Method
tc	769.99	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13170280&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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