

# 3,5-Dimethyl-4-benzyloxyazobenzene

**Inchi:** InChI=1S/C21H20N2O/c1-16-12-17(2)14-20(13-16)23-22-19-8-10-21(11-9-19)24-15-18-6  
**InchiKey:** PEKFOXIPLDGONJ-GHVJWSGMSA-N  
**Formula:** C21H20N2O  
**SMILES:** Cc1cc(C)cc(N=Nc2ccc(OCc3ccccc3)cc2)c1  
**Mol. weight [g/mol]:** 316.40  
**CAS:** 119121-11-8

## Physical Properties

Property code	Value	Unit	Source
chs	-11461.90	kJ/mol	NIST Webbook
hf	113.41	kJ/mol	Joback Method
hfs	340.00	kJ/mol	NIST Webbook
hvap	80.23	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.298		Crippen Method
mcvol	257.000	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
tb	946.48	K	Joback Method
tc	1208.52	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C119121118&Units=SI>  
**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)

## Legend

**chs:** Standard solid enthalpy of combustion

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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