

# 1-(Dimethoxy-phenylmethyl)-1H-imidazole

**Inchi:** InChI=1S/C12H14N2O2/c1-15-12(16-2,14-9-8-13-10-14)11-6-4-3-5-7-11/h3-10H,1-2H3  
**InchiKey:** KDFJJNPLCGDESX-UHFFFAOYSA-N  
**Formula:** C12H14N2O2  
**SMILES:** COC(OC)(c1ccccc1)n1ccnc1  
**Mol. weight [g/mol]:** 218.25  
**CAS:** 111456-85-0

## Physical Properties

Property code	Value	Unit	Source
hf	-77.50 ± 3.70	kJ/mol	NIST Webbook
hfl	-163.10 ± 3.60	kJ/mol	NIST Webbook
hvap	85.60 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.47		Crippen Method
logp	1.834		Crippen Method
mcvol	168.420	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C111456850&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)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hfl:** Liquid phase enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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