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/ci990307l
Crippen Method: 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