6-METHOXYBENZOFUROXAN

Other names: 5-methoxybenzofuroxan
Inchi: InChI=1S/C7H6N2O3/c1-11-5-2-3-6-7(4-5)9(10)12-8-6/h2-4H,1H3
InchiKey: XCWFKHHSXPIDHN-UHFFFAOYSA-N
Formula: C7H6N2O3
SMILES: COc1ccc2no[n+]([O-])c2c1
Mol. weight [g/mol]: 166.14

Physical Properties

Property code	Value	Unit	Source
hf	164.07	kJ/mol	Cheméo Relay (1.0)
logp	0.470		Crippen Method
mcvol	108.140	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3524069&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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