3-Me-phenoxy

Inchi: InChI=1S/C7H7O/c1-6-3-2-4-7(8)5-6/h2-5H,1H3
InchiKey: UGRMITBWUVWUEB-UHFFFAOYSA-N
Formula: C7H7O
SMILES: Cc1cccc([O])c1
Mol. weight [g/mol]: 107.13
CAS: 41115-75-7

Physical Properties

Property code	Value	Unit	Source
affp	877.50	kJ/mol	NIST Webbook
basg	845.00	kJ/mol	NIST Webbook
log10ws	-6.12		Crippen Method
logp	2.139		Crippen Method
mcvol	89.450	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41115757&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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