4-Me-phenoxy

Inchi: InChI=1S/C7H7O/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey: LTKOYWPELWFYHK-UHFFFAOYSA-N
Formula: C7H7O
SMILES: Cc1ccc([O])cc1
Mol. weight [g/mol]: 107.13
CAS: 3174-48-9

Physical Properties

Property code	Value	Unit	Source
affp	884.50	kJ/mol	NIST Webbook
basg	852.00	kJ/mol	NIST Webbook
log10ws	-6.12		Crippen Method
logp	2.139		Crippen Method
mcvol	89.450	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3174489&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from: