Benzenemethanimine, «alpha»-phenyl-N-oxide

Inchi: InChI=1S/C13H11NO/c15-14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,14H
InchiKey: RGGDCZRENGFPSU-UHFFFAOYSA-N
Formula: C13H11NO
SMILES: [O-]N[C+](c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 197.23
CAS: 59862-61-2

Physical Properties

Property code	Value	Unit	Source
ie	7.75	eV	NIST Webbook
log10ws	-4.03		Crippen Method
logp	2.702		Crippen Method
mcvol	158.060	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=C59862612&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.