Methanamine, N-butylidene-, N-oxide

Inchi: InChI=1S/C5H11NO/c1-3-4-5-6(2)7/h5H,3-4H2,1-2H3
InchiKey: YWCNDGABFKKCGI-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CCCC=[N+](C)[O-]
Mol. weight [g/mol]: 101.15
CAS: 44603-43-2

Physical Properties

Property code	Value	Unit	Source
ie	8.57 ± 0.05	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.997		Crippen Method
mcvol	92.860	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C44603432&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

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.