

Sydnone, 3-methyl-

Other names:	3-Methylsydnone
Inchi:	InChI=1S/C3H4N2O2/c1-5-2-3(6)7-4-5/h2H,1H3
InchiKey:	KUYNWZKDWRYCIH-UHFFFAOYSA-N
Formula:	C3H4N2O2
SMILES:	C[n+]1cc([O-])on1
Mol. weight [g/mol]:	100.08
CAS:	6939-12-4

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
log10ws	-9.36		Crippen Method
logp	-1.427		Crippen Method
mcvol	65.370	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=C6939124&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

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<https://www.chemeo.com/cid/42-678-3/Sydnone-3-methyl.pdf>

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