

Sydnone, 3-phenyl-

Other names:	N-Phenylsydnone 3-Phenylsydnone Phenylsydnone 3-Phenylsydnon
Inchi:	InChI=1S/C8H6N2O2/c11-8-6-10(9-12-8)7-4-2-1-3-5-7/h1-6H
InchiKey:	KQEVEDHJIGSXDK-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	[O-]c1c[n+](c2ccccc2)no1
Mol. weight [g/mol]:	162.15
CAS:	120-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.72		Crippen Method
logp	0.025		Crippen Method
mcvol	112.060	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=C120069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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