

Sydnone, diphenyl-

Other names:	Sydnone, 3,4-diphenyl- 3,4-Diphenylsydnone Diphenylsydnone 3,4-Diphenylsydnon
Inchi:	InChI=1S/C14H10N2O2/c17-14-13(11-7-3-1-4-8-11)16(15-18-14)12-9-5-2-6-10-12/h1-10
InchiKey:	PGIGJNLLKIEZGR-UHFFFAOYSA-N
Formula:	C14H10N2O2
SMILES:	[O-]c1on[n+](c2ccccc2)c1-c1ccccc1
Mol. weight [g/mol]:	238.24
CAS:	3815-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.32		Crippen Method
logp	1.692		Crippen Method
mcvol	172.840	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3815836&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

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

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