

Sydnone, 3-(1-methylethyl)-

Other names:	Sydnone, 3-isopropyl- 3-Isopropylsydnone NSC 56786
Inchi:	InChI=1S/C5H8N2O2/c1-4(2)7-3-5(8)9-6-7/h3-4H,1-2H3
InchiKey:	MOPOHDBGHMCTYJK-UHFFFAOYSA-N
Formula:	C5H8N2O2
SMILES:	CC(C)[n+]1cc([O-])on1
Mol. weight [g/mol]:	128.13
CAS:	6939-17-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.71		Crippen Method
logp	-0.383		Crippen Method
mcvol	93.550	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6939179&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-182-5/Sydnone-3-1-methylethyl.pdf>

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