

Aziridine, 1-(2-naphthoyl)-

Inchi:	InChI=1S/C13H11NO/c15-13(14-7-8-14)12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,7-8H2
InchiKey:	BRQKCXRFVLZIPZ-UHFFFAOYSA-N
Formula:	C13H11NO
SMILES:	O=C(c1ccc2ccccc2c1)N1CC1
Mol. weight [g/mol]:	197.23
CAS:	63021-45-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.296		Crippen Method
mcvol	151.500	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63021454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/91-676-1/Aziridine-1-2-naphthoyl.pdf>

Generated by Cheméo on 2024-04-25 19:30:05.885898595 +0000 UTC m=+16362654.806475922.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.