

4-Morpholino-6-methyl-1,3,3a,7-tetrazaindene

Inchi:	InChI=1S/C10H13N5O/c1-8-6-9(14-2-4-16-5-3-14)15-10(13-8)11-7-12-15/h6-7H,2-5H2,1
InchiKey:	WFXJTKDSWVTSJP-UHFFFAOYSA-N
Formula:	C10H13N5O
SMILES:	Cc1cc(N2CCOCC2)n2ncnc2n1
Mol. weight [g/mol]:	219.24
CAS:	78666-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	0.269		Crippen Method
mcvol	157.750	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78666952&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

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