

4-Styrylpyridazine

Inchi:	InChI=1S/C12H10N2/c1-2-4-11(5-3-1)6-7-12-8-9-13-14-10-12/h1-10H/b7-6+
InchiKey:	WHUUTUUXTSPADS-VOTSOKGWSA-N
Formula:	C12H10N2
SMILES:	C(=Cc1ccnnc1)c1ccccc1
Mol. weight [g/mol]:	182.22
CAS:	39816-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.647		Crippen Method
mcvol	148.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39816198&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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