10H-Pyrido(3,2-b)(1,4)benzothiazine

Other names:	1H-Pyrido[3,2-b][1,4]benzothiazine
	Isothipendyl M (ring)
Inchi:	InChI=1S/C11H8N2S/c1-2-5-9-8(4-1)13-11-10(14-9)6-3-7-12-11/h1-7H,(H,12,13)
InchiKey:	UKDZROJJLPDLDO-UHFFFAOYSA-N
Formula:	C11H8N2S
SMILES:	c1ccc2c(c1)Nc1ncccc1S2
Mol. weight [g/mol]:	200.26
CAS:	261-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	3.290		Crippen Method
mcvol	143.780	ml/mol	McGowan Method
rinpol	2045.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2049.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C261961&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

rinpol: Non-polar retention indices