

Pyrimidine, 5-nitro-2-styryl-

Inchi:	InChI=1S/C12H9N3O2/c16-15(17)11-8-13-12(14-9-11)7-6-10-4-2-1-3-5-10/h1-9H/b7-6+
InchiKey:	CMNLEIRGOGWIBG-VOTSOKGWSA-N
Formula:	C12H9N3O2
SMILES:	O=[N+]([O-])c1cnc(C=Cc2ccccc2)nc1
Mol. weight [g/mol]:	227.22
CAS:	54246-65-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	2.555		Crippen Method
mcvol	165.500	ml/mol	McGowan Method

Sources

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=C54246650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/115-133-6/Pyrimidine-5-nitro-2-styryl.pdf>

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