Nocodazole

Other names:	Carbamic acid, [5-(2-thienylcarbonyl)-1H-benzimidazol-2-yl]-, methyl ester Carbamic acid, (5-(2-thienylcarbonyl)-1H-benzimidazole-2-yl)-, methyl ester Methyl (5-(2-thienylcarbonyl)-1H-benzimidazol-2-yl)carbamate Methyl 5-(2-thenoyl)-2-benzimidazolecarbamate Methyl 5-(2-thienoyl)-2-benzimidazolecarbamate Methyl(5-(2-thienylcarbonyl))-1H-benzimidazole-2-yl carbamate N-(5-(2-Thenoyl)-2-benzimidazolyl)carbamic acid methyl ester N-(5-(2-Thienoyl)-2-benzimidazolyl)carbamic acid methyl ester NSC 238159 Oncodazole R 17,934 R 17934 2-Benzimidazolecarbamic acid, 5-(2-thenoyl)-, methyl ester 2-Benzimidazolecarbamic acid, 5-(2-thienoyl)-, methyl ester 2-Benzimidazolecarbamic acid, 5-(2-thienylcarbonyl)-, methyl ester Carbamic acid, N-[5-(2-thenoyl)-1H-benzimidazol-2-yl]-, methyl ester [5-(Thiophene-2-carbonyl)-1H-benzoimidazol-2-yl]-carbamic acid methyl ester Methyl N-(5-thenoyl-2-benzimidazolyl)carbamate [[5-(2-Thienylcarbonyl)-1H-benzimidazol-2-yl]]carbamic acid methyl ester
Inchi:	InChI=1S/C14H11N3O3S/c1-20-14(19)17-13-15-9-5-4-8(7-10(9)16-13)12(18)11-3-2-6-21
InchiKey:	KYRVNWMVYQXFEU-UHFFFAOYSA-N
Formula:	C14H11N3O3S
SMILES:	COC(=O)Nc1nc2cc(C(=O)c3cccs3)ccc2[nH]1
Mol. weight [g/mol]:	301.32
CAS:	31430-18-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	2.552		Crippen Method
mcvol	205.040	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=C31430189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume