METHYL (5-(2-THENOYL)-2-BENZIMIDAZOLYL)CARBAMAT

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]: 301.33

Physical Properties

Property code	Value	Unit	Source
hvap	141.79	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-4.48		Cheméo Relay (1.0)
logp	2.552		Crippen Method
mcvol	205.040	ml/mol	McGowan Method
tf	547.61	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31430189&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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