

methyl

N-[1-(butylcarbamoyl)benzimidazol-2-yl]carbamate

Other names:

1-(Butylcarbamoyl)-2-Benzimidazolecarbamic acid, methyl ester
1-(Butylcarbamoyl)-2-benzimidazol-methylcarbamate
1-(N-Butylcarbamoyl)-2-(methoxy-carboxamido)-benzimidazol
2-Benzimidazolecarbamic acid, 1-(butylcarbamoyl)-, methyl ester
Agrocit
Arilate
BBC
BC 6597
BNM
Benlat
Benlate
Benlate 50
Benlate 50 W
Benomyl 50W
Benomyl-Imex
Carbamic acid, N-(1-((butylamino)carbonyl)-1H-benzimidazol-2-yl)-, methyl ester
Carbamic acid, [1-[(butylamino)carbonyl]-1H-benzimidazol-2-yl]-, methyl ester
D 1991
Du Pont 1991
F 1991
Fundasol
Fundazol
Fungicide 1991
Fungicide D-1991
Fungochrom
Kribenomyl
MBC
Methyl 1-(butylamino)carbonyl-1H-benzimidazol-2-ylcarbamate
Methyl 1-(butylcarbamoyl)-2-benzimidazolecarbamate
Methyl 1-(butylcarbamoyl)-2-benzimidazolylcarbamate
Methyl N-(1-Butylcarbamoyl-2-benzimidazole)carbamate
NS 02
NS 02 (fungicide)
NSC 263489
Tersan 1991
Uzgen
[1-[(Butylamino)carbonyl]-1H-benzimidazol-2-yl]carbamic acid methyl ester
benomyl

Inchi: InChI=1S/C14H18N4O3/c1-3-4-9-15-13(19)18-11-8-6-5-7-10(11)16-12(18)17-14(20)21-2

InchiKey: RIOXQFHNBCKOKP-UHFFFAOYSA-N

Formula: C₁₄H₁₈N₄O₃
SMILES: CCCCNC(=O)n1c(NC(=O)OC)nc2ccccc21
Mol. weight [g/mol]: 290.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Aqueous Solubility Prediction Method
log10ws	-4.88		Estimated Solubility Method
logp	2.572		Crippen Method
mcvol	218.130	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17804352&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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