

Isoxaben

Other names:

Benzamizole
EL 107
Flexidor
Gallery
Knot out
N-[3-(1-Ethyl-1-methylpropyl)-5-isoxazolyl]-2,6-dimethoxybenzamide
NA 8318
Benzamide, N-[3-(1-ethyl-1-methylpropyl)-5-isoxazolyl]-2,6-dimethoxy-
Cent 7
X-Pand

Inchi:

InChI=1S/C18H24N2O4/c1-6-18(3,7-2)14-11-15(24-20-14)19-17(21)16-12(22-4)9-8-10-1

InchiKey:

PMHURSZHKKJGBM-UHFFFAOYSA-N

Formula:

C19H25NO4

SMILES:

CCC(C)(CC)c1cc(NC(=O)c2c(OC)cccc2OC)on1

Mol. weight [g/mol]:

331.41

CAS:

82558-50-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.34		Crippen Method
logp	4.022		Crippen Method
mcvol	260.400	ml/mol	McGowan Method

Sources

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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C82558507&Units=SI>

Legend

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

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