Isocarboxazid

Other names: 1-Benzyl-2-(5-methyl-3-isoxazolylcarbonyl)hydrazine
3-Isoxazolecarboxylic acid, 5-methyl-, 2-(phenylmethyl)hydrazide
3-Isoxazolecarboxylic acid, 5-methyl-, 2-benzylhydrazide
5-Methyl-3-isoxazolecarboxylic acid 2-benzylhydrazide
BMIH
Benazide
Enerzer
Isocarbonazid
Isocarbossazide
Isocarboxazide
Isocarboxyzid
Maraplan
Marplan
Marplon
N'-Benzyl N-methyl-5-isoxazolecarboxylhydrazide-3
NSC 169893
Ro 5-0831
Ro 5-0831/1

Inchi: InChI=1S/C12H13N3O2/c1-9-7-11(15-17-9)12(16)14-13-8-10-5-3-2-4-6-10/h2-7,13H,8H2

InchiKey: XKFPYPQQHFEXRZ-UHFFFAOYSA-N

Formula: C12H13N3O2

SMILES: Cc1cc(C(=O)NNCc2ccccc2)no1

Mol. weight [g/mol]: 231.25

CAS: 59-63-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Aqueous Solubility Prediction Method
log10ws	-2.46		Estimated Solubility Method
logp	1.418		Crippen Method
mcvol	174.100	ml/mol	McGowan Method
rinpol	1960.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1949.00		NIST Webbook

rinpol	1960.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tf	378.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point