Bentranil

Other names:	2-Phenyl-3,1-benzoxazinone-(4) 2-Phenyl-4-[4H]-3,1-benzoxazinone 2-Phenyl-4H-3,1-benzoxazin-4-one 3-Phenyl-1H-2,4-benzoxazin-1-one 3-Phenyl-2,4-benzoxazin-1-one 4H-3,1-Benzoxazin-4-one, 2-phenyl- H-170 Linarotox Linurotox NSC 16082
Inchi:	InChI=1S/C14H9NO2/c16-14-11-8-4-5-9-12(11)15-13(17-14)10-6-2-1-3-7-10/h1-9H
InchiKey:	HTTLBYITFHMYFK-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=c1oc(-c2ccccc2)nc2ccccc12
Mol. weight [g/mol]:	223.23
CAS:	1022-46-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Aqueous Solubility Prediction Method
logp	2.855		Crippen Method
mcvol	162.860	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.70	K	1.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1022464&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure