Brucine

Other names:	(-)-Brucine
	10,11-Dimethoxystrychnine
	10,11-Dimethystrychnine
	2,3-Dimethoxy-strychnine
	2,3-Dimethoxystrychnidine-10-one
	Brucin
	Brucina
	Brucine alkaloid
	Dimethoxy strychnine
	NSC123398
	Rcra waste number P018
	Strychnidin-10-one, 2,3-dimethoxy-
	Strychnine, 2,3-dimethoxy-
	UN 1570
Inchi:	InChI=1S/C23H26N2O4/c1-27-16-8-14-15(9-17(16)28-2)25-20(26)10-18-21-13-7-19-23(1
InchiKey:	RRKTZKIUPZVBMF-UHFFFAOYSA-N
Formula:	C23H26N2O4
SMILES:	COc1cc2c(cc1OC)C13CCN4CC5=CCOC6CC(=O)N2C1C6C5CC43
Mol. weight [g/mol]:	394.46
CAS:	357-57-3

Physical Properties

Property code	Value	Unit	Source
chs	-12270.00	kJ/mol	NIST Webbook
hfs	-496.20	kJ/mol	NIST Webbook
log10ws	-2.09		Aqueous Solubility Prediction Method
logp	2.110		Crippen Method
mcvol	280.850	ml/mol	McGowan Method
rinpol	3310.00		NIST Webbook
rinpol	3310.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C357573&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices