Cytisine

Other names: (-)-Cytisine
1,2,3,4,5,6-Hexahydro-1,5-methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, (1R)-
1,5-Methano-8H-pyrido(1,2-a)(1,5)diazocin-8-one, 1,2,3,4,5,6-hexahydro-
1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R)-
1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R,5S)-
Baptitoxin
Baptitoxine
Citizin
Cystisine
Cytisin
Cytiton
Cytitone
Cytizin
Laburnin
Sophorin
Sophorine
Tabax
Tabex
Tsitizin
Ulexin
Ulexine

Inchi: InChI=1S/C11H14N2O/c14-11-3-1-2-10-9-4-8(5-12-6-9)7-13(10)11/h1-3,8-9,12H,4-7H2

InchiKey: ANJTVLIZGCUXLD-UHFFFAOYSA-N

Formula: C11H14N2O

SMILES: O=c1cccc2n1CC1CNCC2C1

Mol. weight [g/mol]: 190.24

CAS: 485-35-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Aqueous Solubility Prediction Method
logp	0.555		Crippen Method
mcvol	146.200	ml/mol	McGowan Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook

rinpol	1987.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tf	425.65	K	Aqueous Solubility Prediction Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	0.30	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=C485358&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point