PRAZIQUANTEL

Other names:	(+) 2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4H-pyrazino-[2,1-a]isoquinolin-4-one 2-Cyclohexylcarbonyl-1,2,3,6,7,11b-hexahydro-4H-pyrazino(2,1-a)isoquinolin-4-one ((+) praziquantel) 4H-Pyrazino[2,1-a]isoquinolin-4-one, 2-(cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro- Biltricide Cesol Droncit Embay 8440 Pyquiton
Inchi:	InChI=1S/C19H24N2O2/c22-18-13-20(19(23)15-7-2-1-3-8-15)12-17-16-9-5-4-6-14(16)10
InchiKey:	FSVJFNAIGNNGKK-UHFFFAOYSA-N
Formula:	C19H24N2O2
SMILES:	O=C(C1CCCCC1)N1CC(=O)N2CCc3ccccc3C2C1
Mol. weight [g/mol]:	312.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Aqueous Solubility Prediction Method
logp	2.535		Crippen Method
mcvol	245.330	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.80	kJ/mol	412.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55268741&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume