Disopyramide

Other names:

2-Pyridineacetamide, «alpha»-[2-(diisopropylamino)ethyl]-«alpha»-phenyl-

2-Pyridineacetamide, «alpha»-[2-[bis(1-methylethyl)amino]ethyl]-«alpha»-phenyl-

2-Pyridineacetamide, Â«alphaÂ»-[2-(diisopropylamino)ethyl]-Â«alphaÂ»-phenyl-

2-Pyridineacetamide, Â«alphaÂ»-[2-[bis(1-methylethyl)amino]ethyl]-Â«alphaÂ»-phenyl-

4-Diisopropylamino-2-phenyl-2-(2-pyridyl)-butyramide

Dicorantil

H 3292

Isorythm

Lispine

Ritmodan

Rythmodan

SC 7031

Searle 703

«alpha»-(2-(Diisopropylamino)ethyl)-«alpha»-phenyl-2-pyridineacetamide

«alpha»-[2-[bis(1-methylethyl)amino]ethyl]-«alpha»-phenyl-2-pyridineacetamide (disopyramide)

«gamma»-Diisopropylamino-«alpha»-phenyl-«alpha»-(2-pyridyl)butyramide

Â«alphaÂ»-(2-(Diisopropylamino)ethyl)-Â«alphaÂ»-phenyl-2-pyridineacetamide

Â«alphaÂ»-[2-[bis(1-methylethyl)amino]ethyl]-Â«alphaÂ»-phenyl-2-pyridineacetamide (disopyramide)

Â«gammaÂ»-Diisopropylamino-Â«alphaÂ»-phenyl-Â«alphaÂ»-(2-pyridyl)butyramide

Inchi: InChI=1S/C21H29N3O/c1-16(2)24(17(3)4)15-13-21(20(22)25,18-10-6-5-7-11-18)19-12-8

InchiKey: UVTNFZQICZKOEM-UHFFFAOYSA-N

Formula: C21H29N3O

SMILES: CC(C)N(CCC(C(N)=O)(c1ccccc1)c1ccccn1)C(C)C

Mol. weight [g/mol]: 339.47

CAS: 3737-09-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Aqueous Solubility Prediction Method
log10ws	-1.70		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.362		Crippen Method
mcvol	290.740	ml/mol	McGowan Method
rinpol	2490.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2566.10		NIST Webbook

rinpol	2525.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2489.00		NIST Webbook
tf	367.93	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.70	kJ/mol	363.70	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3737095&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

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point