Furazabol

Inchi: InChI=1S/C20H30N2O2/c1-18-11-17-16(21-24-22-17)10-12(18)4-5-13-14(18)6-8-19(2)15

InchiKey: RGLLOUBXMOGLDQ-UTOPOAIZSA-N

Formula: C20H30N2O2

SMILES: CC12Cc3nonc3CC1CCC1C2CCC2(C)C1CCC2(C)O

Mol. weight [g/mol]: 330.46

CAS: 1239-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.71		Crippen Method
logp	3.778		Crippen Method
mcvol	261.460	ml/mol	McGowan Method
rinpol	2895.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1239298&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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