Fominoben

Inchi: InChI=1S/C21H24ClN3O3/c1-24(15-20(26)25-10-12-28-13-11-25)14-17-18(22)8-5-9-19(
InchiKey: KSNNEUZOAFRTDS-UHFFFAOYSA-N
Formula: C21H24ClN3O3
SMILES: CN(CC(=O)N1CCOCC1)Cc1c(Cl)cccc1NC(=O)c1ccccc1
Mol. weight [g/mol]: 401.89
CAS: 18053-31-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.883		Crippen Method
mcvol	299.560	ml/mol	McGowan Method
rinpol	3210.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18053311&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.