FENAZAQUIN

Other names: 4-[2-(4-tert-Butylphenyl)ethoxy]quinazoline
Quinazoline, 4-[2-[4-(1,1-dimethylethyl)phenyl]ethoxy]-
Inchi: InChI=1S/C20H22N2O/c1-20(2,3)16-10-8-15(9-11-16)12-13-23-19-17-6-4-5-7-18(17)21-
InchiKey: DMYHGDXADUDKCQ-UHFFFAOYSA-N
Formula: C20H22N2O
SMILES: CC(C)(C)c1ccc(CCOc2ncnc3ccccc23)cc1
Mol. weight [g/mol]: 306.40
CAS: 120928-09-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.549		Crippen Method
mcvol	251.510	ml/mol	McGowan Method
rinpol	2499.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120928098&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices