

2-Hydroxyethylflurazepam, trimethylsilyl ether

Inchi: InChI=1S/C20H22ClFN2O2Si/c1-27(2,3)26-11-10-24-18-9-8-14(21)12-16(18)20(23-13-14)22
InchiKey: KKSGIGSWBKIJGJ-UHFFFAOYSA-N
Formula: C₂₀H₂₂ClFN₂O₂Si
SMILES: C[Si](C)(C)OCCN1C(=O)CN=C(c2ccccc2F)c2cc(Cl)ccc21
Mol. weight [g/mol]: 404.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	4.515		Crippen Method
rinsol	2701.80		NIST Webbook
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Sources

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417198&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/87-443-4/2-Hydroxyethylflurazepam-trimethylsilyl-ether.pdf>

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