

Inabenfide, N,O-bis(trimethylsilyl)-

Inchi: InChI=1S/C25H31ClN2O2Si2/c1-31(2,3)28(25(29)20-14-16-27-17-15-20)23-13-12-21(26)
InchiKey: ISBVUOUPPNNVAA-UHFFFAOYSA-N
Formula: C25H31ClN2O2Si2
SMILES: C[Si](C)(C)OC(c1cccc1)c1cc(Cl)ccc1N(C(=O)c1ccncc1)[Si](C)(C)C
Mol. weight [g/mol]: 483.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	7.158		Crippen Method
rinpol	2710.20		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U334042&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/15-977-1/Inabenfide-N-O-bis-trimethylsilyl.pdf>

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