Pentazocine, trimethylsilyl ether

Inchi: InChI=1S/C22H35NOSi/c1-16(2)10-12-23-13-11-22(4)17(3)21(23)14-18-8-9-19(15-20(18
InchiKey: KMKNLGHEFMHPCX-UHFFFAOYSA-N
Formula: C22H35NOSi
SMILES: CC(C)=CCN1CCC2(C)c3cc(O[Si](C)(C)C)ccc3CC1C2C
Mol. weight [g/mol]: 357.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	5.391		Crippen Method
rinpol	2282.60		NIST Webbook
rinpol	2282.60		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U417223&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
rinpol: Non-polar retention indices