Pentazocine tms derivative

Other names: Pentazocine O-TMS
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]: 357.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Cheméo Relay (1.0)
logp	5.391		Crippen Method
tf	383.43	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U137224&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
tf: Normal melting (fusion) point