

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

Latest version available from:

<https://www.chemeo.com/cid/84-477-0/Pentazocine-tms-derivative.pdf>

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