

Thiethylperazine M (sulfone)

Inchi: InChI=1S/C22H29N3OS2/c1-3-28(26)18-9-10-22-20(17-18)25(19-7-4-5-8-21(19)27-22)1.
InchiKey: MBXPSQGCQPTXKD-UHFFFAOYSA-N
Formula: C22H29N3OS2
SMILES: CCS(=O)c1ccc2c(c1)N(CCCN1CCN(C)CC1)c1ccccc1S2
Mol. weight [g/mol]: 415.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	4.054		Crippen Method
mcvol	320.110	ml/mol	McGowan Method
rinpol	3400.00		NIST Webbook
rinpol	3400.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314548&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/39-692-1/Thiethylperazine-M-sulfone.pdf>

Generated by Cheméo on 2025-12-05 13:55:14.527957392 +0000 UTC m=+4691112.057998056.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.