

Dixyrazine

Other names:	Ethanol, 2-[2-[4-[2-methyl-3-(10H-phenothiazin-10-yl)propyl]-1-piperazinyl]ethoxy]- Ethanol, 2-[2-[4-(2-methyl-3-phenothiazin-10-ylpropyl)-1-piperazinyl]ethoxy]- Esocalm Esucos Metronal Roscal U. C. B. 3412 UCB 3412 10-(3-(4-Hydroxyethoxyethyl-1-piperazinyl)-2-methylpropyl)phenothiazine (2-Methyl-3-(1-hydroxyethoxyethyl-4-piperazinyl)propyl)-10-phenothiazine 2-(2-(4-(2-Methyl-3-phenothiazin-10-ylpropyl)-1-piperazinyl)ethoxy)ethanol 2-[2-[4-[2-methyl-3-(10H-phenothiazin-10-yl)propyl]piperazin-1-yl]ethoxy]ethanol
Inchi:	InChI=1S/C24H33N3O2S/c1-20(18-26-12-10-25(11-13-26)14-16-29-17-15-28)19-27-21-
InchiKey:	MSYUMPGNGDNTIQ-UHFFFAOYSA-N
Formula:	C24H33N3O2S
SMILES:	CC(CN1CCN(CCOCCO)CC1)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	427.60
CAS:	2470-73-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.552		Crippen Method
mcvol	337.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2470737&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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