Alimemazine M (hydroxy-), acetylated

Other names: Alimemazine M (hydroxy-), acetylated
Inchi: InChI=1S/C20H24N2O2S/c1-14(12-21(3)4)13-22-17-7-5-6-8-19(17)25-20-11-16(24-15(2)
InchiKey: ZQAKZDUDVCBPBB-UHFFFAOYSA-N
Formula: C20H24N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC(C)CN(C)C
Mol. weight [g/mol]: 356.49

Physical Properties

Property code	Value	Unit	Source
ie	6.76	eV	Cheméo Relay (1.0)
log10ws	-4.83		Cheméo Relay (1.0)
logp	4.412		Crippen Method
mcvol	278.030	ml/mol	McGowan Method
rinpol	2600.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tf	415.57	K	Cheméo Relay (1.0)

Sources

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=R310135&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point