

10H-Phenothiazine-10-propanamine, 2-methoxy-N,N-dimethyl-

Other names:

10H-Phenothiazine-10-propanamine, 2-methoxy-N,N-dimethyl-
Phenothiazine, 10-[3-(dimethylamino)propyl]-2-methoxy-
Methopromazine
Tenton
Tentone
10-[3-(Dimethylamino)propyl]-2-methoxyphenothiazine
2-Methoxy-10-[3'-(dimethylamino)propyl]phenothiazine
2-Methoxypromazine
4632 R.P
Neoproma
RP 4632
2-Methoxy-N,N-dimethyl-10H-phenothiazine-10-propanamine

Inchi: InChI=1S/C18H22N2OS/c1-19(2)11-6-12-20-15-7-4-5-8-17(15)22-18-10-9-14(21-3)13-16
InchiKey: BRABPYPSZVCCCLR-UHFFFAOYSA-N
Formula: C18H22N2OS
SMILES: COc1ccc2c(c1)N(CCCN(C)C)c1ccccc1S2
Mol. weight [g/mol]: 314.45

Physical Properties

Property code	Value	Unit	Source
ie	7.23	eV	Cheméo Relay (1.0)
log10ws	-4.60		Cheméo Relay (1.0)
logp	4.250		Crippen Method
mcvol	248.280	ml/mol	McGowan Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tf	396.52	K	Cheméo Relay (1.0)

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C61018&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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