Ethanone, 1-[10-[3-(dimethylamino)propyl]-10H-phenothiazin

Other names: Ethanone, 1-[10-[3-(dimethylamino)propyl]-10H-phenothiazin-2-yl]-
Ketone, 10-[3-(dimethylamino)propyl]phenothiazin-2-yl methyl
Acepromazin
Acetacin
Acetazin
Acetazine
Acetopromazine
Acetylpromazine
Azapromazine
Azepromazine
Notensil
Plegicil
Plivafen
Vetranquil
10-(3-Dimethylaminopropyl)phenothiazin-3-yl methyl ketone
1522 C. B.
1522CB
2-Acetyl-10-[3-(Dimethylamino)propyl]phenylthiazine
2-Acetylpromazine
3-Acetyl-10-(3-dimethylaminopropyl)phenothiazine
Acepromazina
Acepromizina
Acetilpromazina
2-Acetyl-10-(3-dimethylaminopropyl)phenothiazine
Acetylpromazin
3-Acetyl-promazin
Atsetozin
AY-57,062
10-(3-Dimethylaminopropyl)phenothiazine-3-ethanone
1-(10-(3-(Dimethylamino)propyl)-10H-phenothiazin-2-yl)ethanone
Plivaphen
Promazine, acetyl-
SV-1522
Vetranquill
WY-1172
10-[3-(Dimethylamino)propyl]-10H-phenothiazin-2-yl methyl ketone

Inchi: InChI=1S/C19H22N2OS/c1-14(22)15-9-10-19-17(13-15)21(12-6-11-20(2)3)16-7-4-5-8-18

InchiKey: NOSIYYJFMPDDSA-UHFFFAOYSA-N

Formula: C19H22N2OS

SMILES: CC(=O)c1ccc2c(c1)N(CCCN(C)C)c1ccccc1S2

Mol. weight [g/mol]: 326.46

Physical Properties

Property code	Value	Unit	Source
ie	7.52	eV	Cheméo Relay (1.0)
log10ws	-4.42		Cheméo Relay (1.0)
logp	4.444		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
rinpol	2720.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2713.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2713.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tf	419.91	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	489.00 ± 1.00	K	0.07	NIST Webbook
tbrp	482.00 ± 1.00	K	0.01	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61007&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point