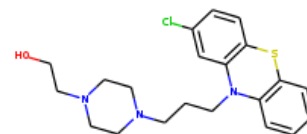


Perphenazine

Other names:

1',1-(2-Idrossietil)-4,3-(2-cloro-10-fenotiazil)propilpiperazina;
1-(2-Hydroxyethyl)-4-(3-(2-chloro-10-phenothiazinyl)propyl)piperazine;
1-Piperazineethanol, 4-[3-(2-Chlorophenothiazin-10-yl)propyl]-;
1-Piperazineethanol, 4-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-;
2-Chloro-10-(3-(4-(2-hydroxyethyl)piperazin-1-yl)propyl)phenothiazine;
2-Chloro-10-3-(1-(2-hydroxyethyl)-4-piperazinyl)propyl phenothiazine;
4-(3-(2-Chlorophenothiazin-10-yl)propyl)-1-piperazineethanol;
Chlorperphenazine; Decentan; Emesinal; Etaperazin; Etaperazine;
Ethaperazine; F-mon; Fentazin; NSC 150866; PZC; Perfenazina;
Perfenazine; Perfenil; Perphenan; Perphenazin; Piperazineethanol,
4-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-; Sch 3940; Thilatazin;
Tranquisan; Trifaron; Trilafon; Trilifan; Triphenot; «gamma»-(4-(«beta»-Hydroxyethyl)piperazin-1-yl)propyl-2-chlorophenothiazine.



InChI: InChI=1S/C21H26ClN3OS/c22-17-6-7-21-19(16-17)25(18-4-1-2-5-20(18)27-21)9-3-8-23-10-12-24(13-11-23)14-15-26/h1-2,4-7,16,26H,3,8-15H2

InChI Key: RGCVKNLCSQQDEP-UHFFFAOYSA-N

Formula: C₂₁H₂₆ClN₃OS

SMILES: OCCN1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1

Molecular Weight: 403.97

CAS: 58-39-9

Physical Properties

Property	Value	Unit	Source
IE	8.63 ± 0.07	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	3.94		Crippen Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$\Delta_{\text{fus}}H$	41.80	kJ/mol	370.0	NIST Webbook

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H26ClN3OS/c22-17-6-7-21-19\(16-17\)25\(18-4-1-2-5-20\(18\)27-21\)9-3-8-23-10-12-24\(13-11-23\)14-15-26/h1-2,4-7,16,26H,3,8-15H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H26ClN3OS/c22-17-6-7-21-19(16-17)25(18-4-1-2-5-20(18)27-21)9-3-8-23-10-12-24(13-11-23)14-15-26/h1-2,4-7,16,26H,3,8-15H2)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_{\text{fus}}H$: Enthalpy of fusion at a given temperature (kJ/mol).

IE: Ionization energy (eV).

logP_{oct/wat}: Octanol/Water partition coefficient .

Latest version available from:

<https://www.cheméo.com/cid/62-333-3/Perphenazine>

Generated by **Cheméo** on Mon, 27 May 2019 01:28:54 +0000.

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