Chlorpromazine

Other names:

10H-Phenothiazine-10-propanamine, 2-chloro-N,N-dimethyl-
2-Chloro-10-[3-(Dimethylamino)propyl]phenothiazine
2-Chloropromazine
2-Cloro-10 (3-dimetilaminopropil)fenotiazina
2601-A
4560 R.P.
Aminasine
Aminazin
Aminazine
Ampliactil
Amplicitil
Amplictil
BC 135
CPZ
Chlor-Promanyl
Chlorderazin
Chloropromazine
Chlorpromados
Chlorpromazin
Clorpromazina
Contomin
Elmarin
Esmind
Fenactil
Fenaktyl
Fraction AB
HL 5746
Largactil
Largactilothiazine
Largactyl
Megaphen
Novomazina
Phenactyl
Phenothiazine, 2-chloro-10-[3-(dimethylamino)propyl]-
Plegomasine
Proma
Promactil
Promazil
Propaphenin
Prozil

	Psychozine
	RP-4560
	SKF 2601-A
	Sanopron
	Thorazine
	Torazina
	Wintermin
Inchi:	InChI=1S/C17H19ClN2S/c1-19(2)10-5-11-20-14-6-3-4-7-16(14)21-17-9-8-13(18)12-15(1
InchiKey:	ZPEIMTDSQAKGNT-UHFFFAOYSA-N
Formula:	C17H19ClN2S
SMILES:	CN(C)CCCN1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]:	318.86
CAS:	50-53-3

Physical Properties

Property code	Value	Unit	Source
ie	7.16 ± 0.08	eV	NIST Webbook
ie	7.38 ± 0.13	eV	NIST Webbook
ie	8.25 ± 0.07	eV	NIST Webbook
log10ws	-5.07		Aqueous Solubility Prediction Method
logp	4.894		Crippen Method
mcvol	240.560	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2538.00		NIST Webbook
rinpol	2487.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2490.00		NIST Webbook

rinpol	2490.00	NIST Webbook
rinpol	2490.00	NIST Webbook
rinpol	2480.00	NIST Webbook
rinpol	2486.00	NIST Webbook
rinpol	2480.00	NIST Webbook
rinpol	2440.00	NIST Webbook
rinpol	2486.00	NIST Webbook
rinpol	2440.00	NIST Webbook
rinpol	2515.00	NIST Webbook
rinpol	2499.00	NIST Webbook
rinpol	2525.00	NIST Webbook
rinpol	2452.00	NIST Webbook
rinpol	2487.00	NIST Webbook
rinpol	2500.00	NIST Webbook
rinpol	2525.00	NIST Webbook
rinpol	2540.00	NIST Webbook
rinpol	2499.00	NIST Webbook
rinpol	2525.00	NIST Webbook
rinpol	2526.00	NIST Webbook
rinpol	2479.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	475.70	K	0.10	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50533&Units=SI
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
tbrp:	Boiling point at reduced pressure