Chlorprothixene

Other names:

(Z)-2-Chloro-N,N-dimethylthioxanthene-«DELTA»9,«gamma»-propylamine
(Z)-2-Chloro-N,N-dimethylthioxanthene-Â«DELTAÂ»9,Â«gammaÂ»-propylamine
1-Propanamine, 3-(2-chloro-9H-thioxanthen-9-ylidene)-N,N-dimethyl-, (Z)-
2-Chloro-9-(3-(dimethylamino)propylidene)thioxanthene, (Z)-
2-Chloro-N,N-dimethylthioxanthene-«DELTA»9,«gamma»-propylamine
2-Chloro-N,N-dimethylthioxanthene-Â«DELTAÂ»9,Â«gammaÂ»-propylamine
9H-Thioxanthene, 1-propanamine deriv.
CPT
CPX
Chloroprothixene
Chlorprothixen
Chlorprothixine
Chlorprotixen
Chlorprotixene
Chlothixen
Iaractan
MK 184
N 714
N 714C
Paxyl
Rentovet
Ro 4-0403
Ro-4-04033
Tactaran
Taractan
Tarasan
Tardan
Thioxanthene-«DELTA»9, «gamma»-propylamine, 2-chloro-N,N-dimethyl-
Thioxanthene-«DELTA»9,«gamma»-propylamine, 2-chloro-N,N-dimethyl-, (Z)-
Thioxanthene-Â«DELTAÂ»9, Â«gammaÂ»-propylamine, 2-chloro-N,N-dimethyl-
Thioxanthene-Â«DELTAÂ»9,Â«gammaÂ»-propylamine, 2-chloro-N,N-dimethyl-, (Z)-
Tranquilan
Trictal
Truxal
Truxaletten
Truxil
Vetacalm
cis-2-Chloro-9-(3-dimethylaminopropylidene)thioxanthene
cis-Chlorprothixene
«alpha»-Chlorprothixene

	Â«alphaÂ»-Chlorprothixene
Inchi:	InChI=1S/C18H18ClNS/c1-20(2)11-5-7-14-15-6-3-4-8-17(15)21-18-10-9-13(19)12-16(14)
InchiKey:	WSPOMRSOLSGNFJ-VGOFMYFVSA-N
Formula:	C18H18ClS
SMILES:	CN(C)CCC=C1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]:	301.85
CAS:	113-59-7

Physical Properties

Property code	Value	Unit	Source
gf	561.34	kJ/mol	Joback Method
hf	296.18	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
ie	7.68 ± 0.03	eV	NIST Webbook
log10ws	-6.74		Aqueous Solubility Prediction Method
logp	5.188		Crippen Method
mcvol	240.370	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2452.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2487.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2487.00		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2487.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	791.02	K	Joback Method
tc	1036.18	K	Joback Method
tf	370.30 ± 0.20	K	NIST Webbook
tf	602.55	K	Aqueous Solubility Prediction Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.37	J/mol×K	995.32	Joback Method
cpg	643.46	J/mol×K	791.02	Joback Method
cpg	658.38	J/mol×K	831.88	Joback Method
cpg	672.37	J/mol×K	872.74	Joback Method
cpg	685.59	J/mol×K	913.60	Joback Method
cpg	698.20	J/mol×K	954.46	Joback Method
cpg	722.25	J/mol×K	1036.18	Joback Method
hfust	27.82	kJ/mol	370.30	NIST Webbook
hfust	27.82	kJ/mol	370.30	NIST Webbook
hfust	28.90	kJ/mol	370.50	NIST Webbook
sfust	75.10	J/mol×K	370.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C113597&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume