

Trietazine

Other names:

1,3,5-Triazine-2,4-diamine, 6-chloro-N,N,N'-triethyl-
1,3,5-Triazine-2,4-diamine, 6-chloro-N₂,N₂,N₄-triethyl-
2-Chloro-4-(diethylamino)-6-(ethylamino)-s-triazine
2-Chloro-4-ethylamino-6-diethylamino-s-triazine
2-Ethylamino-4-Diethylamino-6-chlorotriazine
2-Ethylamino-4-diethylamino-6-chloro-s-triazine
6-Chloro-N,N,N'-triethyl-1,3,5-triazine-2,4-diamine
Aventox
Bronox
G 27901
Gesafloc
NC 1667
NSC 13908
Rental
Triethazine
s-Triazine, 2-chloro-4-(diethylamino)-6-(ethylamino)-

Inchi: InChI=1S/C9H16ClN5/c1-4-11-8-12-7(10)13-9(14-8)15(5-2)6-3/h4-6H2,1-3H3,(H,11,12,1**InchiKey:** HFBWPRKWDIRYNX-UHFFFAOYSA-N**Formula:** C₉H₁₆ClN₅**SMILES:** CCNc1nc(Cl)nc(N(CC)CC)n1**Mol. weight [g/mol]:** 229.71**CAS:** 1912-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Estimated Solubility Method
log10ws	-4.06		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
rinpol	1760.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
ripol	2557.00		NIST Webbook

ripol	2559.00	NIST Webbook
ripol	2557.00	NIST Webbook
ripol	2557.00	NIST Webbook
ripol	2557.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912261&Units=SI>

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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