1,3,5-Triazine-2,4-diamine, 6-chloro-N,N,N',N'-tetraethyl-

Other names: 2,4-Bis(diethylamino)-6-chloro-1,3,5-triazine
2,4-Bis(diethylamino)-6-chloro-s-triazine
2-Chloro-4,6-bis(diethylamino)-s-triazine
2-chloro-4,6-bis(diethylamino)-1,3,5-triazine
6-Chloro-N,N,N',N'-tetraethyl-1,3,5-triazine-2,4-diamine
Chlorazin
Chlorazine
Chloroazine
G 25,804
G 444E
Geigy 444E
Geigy Herbicide 444E
NSC 56355
NSC 56840
Phenazon
s-Triazine, 2-chloro-4,6-bis(diethylamino)-

Inchi: InChI=1S/C11H20ClN5/c1-5-16(6-2)10-13-9(12)14-11(15-10)17(7-3)8-4/h5-8H2,1-4H3

InchiKey: QHXDTLYEHWXDSO-UHFFFAOYSA-N

Formula: C11H20ClN5

SMILES: CCN(CC)c1nc(Cl)nc(N(CC)CC)n1

Mol. weight [g/mol]: 257.76

CAS: 580-48-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Aqueous Solubility Prediction Method
log10ws	-4.41		Estimated Solubility Method
logp	2.217		Crippen Method
mcvol	204.230	ml/mol	McGowan Method
ripol	2309.00		NIST Webbook

Sources

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=C580483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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