Atraton

Other names:	1,3,5-Triazine-2,4-diamine, N-ethyl-6-methoxy-N'-(1-methylethyl)-
	1,3,5-Triazine-2,4-diamine, N2-ethyl-6-methoxy-N4-(1-methylethyl)-
	2-(Ethylamino)-4-(isopropylamino)-6-methoxy-s-triazine
	2-Methoxy-4-ethylamino-6-isopropylamino-1,3,5-triazine
	2-Methoxy-4-ethylamino-6-isopropylamino-s-triazine
	2-Methoxy-4-isopropylamino-6-ethylamino-s-triazine
	4-Ethylamino-6-isopropylamino-2-methoxy-s-triazine
	6-Ethylamino-4-isopropylamino-2-methoxy-1,3,5-triazine
	Atratone
	Atroton
	G 32293
	Geigy 32,293
	Gesatamin
	N-Ethyl-6-methoxy-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine
	NSC 163045
	Primatol
	s-Triazine, 2-(ethylamino)-4-(isopropylamino)-6-methoxy-
	s-Triazine, 4-ethylamino-6-isopropylamino-2-methoxy-
Inchi:	InChI=1S/C9H17N5O/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11
InchiKey:	PXWUKZGIHQRDHL-UHFFFAOYSA-N
Formula:	C9H17N5O
SMILES:	CCNc1nc(NC(C)C)nc(OC)n1
Mol. weight [g/mol]:	211.26
CAS:	1610-17-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Aqueous Solubility Prediction Method
log10ws	-2.08		Estimated Solubility Method
logp	1.132		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
ripol	2633.00		NIST Webbook
ripol	2610.00		NIST Webbook
ripol	2610.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	94.40	kJ/mol	363.00	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=C1610179&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

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices