

Cyanazine

Other names:

Propanenitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl-
Propionitrile, 2-[[4-chloro-6-(ethylamino)-s-triazin-2-yl]amino]-2-methyl-
Bladex
Bladex 80WP
DW 3418
SD 15418
WL 19805
2-[[4-Chloro-6-(ethylamino)-s-triazin-2-yl]amino]-2-methylpropionitrile
Fortol
Fortrol
Payze
Propionitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl
S-Triazine, 2-chloro-4-(ethylamino)-6-(1-cyano-1-methyl)(ethylamino)-
2-Chloro-4-(1-cyano-1-methylethylamino)-6-ethylamino-s-triazine
Cyanazin

Inchi:

InChI=1S/C9H13ClN6/c1-4-12-7-13-6(10)14-8(15-7)16-9(2,3)5-11/h4H2,1-3H3,(H2,12,13)

InchiKey:

MZZBPKVEFVLFF-UHFFFAOYSA-N

Formula:

C9H13ClN6

SMILES:

CCN=c1nc(Cl)nc(NC(C)(C)C#N)[nH]1

Mol. weight [g/mol]:

240.69

CAS:

11096-88-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	0.611		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
rinpol	1951.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	333.91		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	333.91		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C11096881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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