

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 2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile
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:	MZZBPDKVEFVLFF-UHFFFAOYSA-N
Formula:	C9H13ClN6
SMILES:	CCN=c1nc(Cl)nc(NC(C)(C)C#N)[nH]1
Mol. weight [g/mol]:	240.69
CAS:	21725-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	0.611		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
tf	438.74 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hfust	41.96	kJ/mol	437.90	NIST Webbook
hsubt	90.70	kJ/mol	352.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C21725462&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point

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