

Terbuthylazine

Other names:	1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylethyl)-N'-ethyl-s-Triazine, 2-(tert-butylamino)-4-chloro-6-(ethylamino)- G 13529 Gardoprim GS 13529 Terbutylethylazine 2-Chloro-4-(Ethylamino)-6-(tert-butylamino)-s-triazine 2-t-Butylamino-4-chloro-6-ethylamino-1,3,5-triazine Primatol M Tyllanex N-tert-Butyl-6-chloro-N'-ethyl-[1,3,5]triazin-2,4-diamin N-tert-Butyl-6-chloro-N'-ethyl-[1,3,5]triazin-2,4-diamine Terbutylazine s-Triazine, 2-chloro-4-ethylamino-6-(1,1-dimethylethyl)amino Terbuthylazin 1,3,5-Triazine-2,4-diamine, 6-chloro-N2-(1,1-dimethylethyl)-N4-ethyl- 2-Chloro-4-tert-butylamino-6-ethylamino-s-triazine 2-tert-Butylamino-4-chloro-6-ethylamino-s-triazine ChlorCaragard Gardeprim A 1862 Terbutazine 6-Chloro-N-(1,1-dimethylethyl)-N'-ethyl-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C9H16ClN5/c1-5-11-7-12-6(10)13-8(14-7)15-9(2,3)4/h5H2,1-4H3,(H2,11,12,13
InchiKey:	FZXISNSWEXTPMF-UHFFFAOYSA-N
Formula:	C9H16ClN5
SMILES:	CCNc1nc(Cl)nc(NC(C)(C)C)n1
Mol. weight [g/mol]:	229.71
CAS:	5915-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.167		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
rinpol	1779.00		NIST Webbook
rinpol	1773.00		NIST Webbook

rinpol	1754.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	298.87		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1785.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2686.00		NIST Webbook
ripol	2664.00		NIST Webbook
tf	449.23 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.57	kJ/mol	448.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5915413&Units=SI
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

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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