

1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(1-methylpropyl)-

Other names:	s-Triazine, 2-(sec-butylamino)-4-chloro-6-(ethylamino)- 2-Aethylamino-4-sek.butylamino-6-chlor-1,3,5-triazin GS 13528 Sebuthylazine Sebutylazine
Inchi:	InChI=1S/C9H16ClN5/c1-4-6(3)12-9-14-7(10)13-8(15-9)11-5-2/h6H,4-5H2,1-3H3,(H2,11)
InchiKey:	BZRUVKZGXNSXMB-UHFFFAOYSA-N
Formula:	C9H16ClN5
SMILES:	CCNc1nc(Cl)nc(NC(C)CC)n1
Mol. weight [g/mol]:	229.71
CAS:	7286-69-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.167		Crippen Method
mcvol	176.050	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7286693&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/55-569-0/1-3-5-Triazine-2-4-diamine-6-chloro-N-ethyl-N-1-methylpropyl.pdf>

Generated by Cheméo on 2024-04-26 15:53:34.383337085 +0000 UTC m=+16436063.303914400.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.