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/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=C7286693&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume