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

Other names: 2-Aethylamino-4-sek.butylamino-6-chlor-1,3,5-triazin
6-chloro-N-ethyl-N'-(1-methylpropyl)-1,3,5-triazine-2,4-diamine
GS 13528
Sebuthylazine
Sebutylazine
s-Triazine, 2-(sec-butylamino)-4-chloro-6-(ethylamino)-

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]: 229.72

Physical Properties

Property code	Value	Unit	Source
hf	-62.05	kJ/mol	Cheméo Relay (1.0)
hvap	105.98	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.22		Cheméo Relay (1.0)
logp	2.167		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
tf	386.09	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Octanol/Water Partition Coefficient of Selected Herbicides: Determination Using Shake-Flask Method and Reversed-Phase High-Performance Liquid Chromatography: https://www.doi.org/10.1021/je049947x

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7286693&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point