

Pyridin-4-amine, 3,5-dichloro-2-trichloromethyl-

Other names: 4-Amino-3,5-dichloro-2-(trichloromethyl)pyridine
Inchi: InChI=1S/C6H3Cl5N2/c7-2-1-13-5(6(9,10)11)3(8)4(2)12/h1H,(H2,12,13)
InchiKey: WEYZLTAYNCBWFU-UHFFFAOYSA-N
Formula: C6H3Cl5N2
SMILES: Nc1c(Cl)cnc(C(Cl)(Cl)Cl)c1Cl
Mol. weight [g/mol]: 280.37
CAS: 14321-05-2

Physical Properties

Property code	Value	Unit	Source
chs	-2726.20	kJ/mol	NIST Webbook
hfs	-181.50	kJ/mol	NIST Webbook
log10ws	-4.24		Crippen Method
logp	3.797		Crippen Method
mcvol	152.800	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14321052&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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