2-Amino-4-anilino-6-(chloromethyl)-s-triazine

Inchi: InChI=1S/C10H10ClN5/c11-6-8-14-9(12)16-10(15-8)13-7-4-2-1-3-5-7/h1-5H,6H2,(H3,12,

InchiKey: ZEXYPLRLARKYLF-UHFFFAOYSA-N

Formula: C10H10ClN5

SMILES: N=c1nc(CCl)[nH]c(=Nc2ccccc2)[nH]1

Mol. weight [g/mol]: 235.67

CAS: 30355-60-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	0.225		Crippen Method
mcvol	166.380	ml/mol	McGowan Method

Sources

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=C30355603&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume