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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30355603&Units=SI
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

Legend

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

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