

9H-Purine-9-acetic acid, 6-[(p-chlorophenyl)amino]-, ethyl ester

Other names:	Ethyl 9-[6-p-chloroanilino]purineacetate
Inchi:	InChI=1S/C15H14ClN5O2/c1-2-23-12(22)7-21-9-19-13-14(17-8-18-15(13)21)20-11-5-3-1
InchiKey:	GRZHGZVUENNXNQ-UHFFFAOYSA-N
Formula:	C15H14ClN5O2
SMILES:	CCOC(=O)Cn1cnc2c(Nc3ccc(Cl)cc3)ncnc21
Mol. weight [g/mol]:	331.76
CAS:	101103-22-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	2.786		Crippen Method
mcvol	229.110	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101103224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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