Triazolo[4,5-d]pyrimidine, 1h-v-, 5,7-dichloro

Inchi: InChI=1S/C4HCl2N5/c5-2-1-3(10-11-9-1)8-4(6)7-2/h(H,7,8,9,10,11)
InchiKey: ZHCMLGWKJKQHTQ-UHFFFAOYSA-N
Formula: C4HCl2N5
SMILES: Clc1nc(Cl)c2nn[nH]c2n1
Mol. weight [g/mol]: 189.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	0.573		Crippen Method
mcvol	102.680	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008681&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