Pyrimidine, 4,6-dichloro-2-ethyl-5-nitro-

Inchi: InChI=1S/C6H5Cl2N3O2/c1-2-3-9-5(7)4(11(12)13)6(8)10-3/h2H2,1H3
InchiKey: RBGNCLAOWBJWLD-UHFFFAOYSA-N
Formula: C6H5Cl2N3O2
SMILES: CCc1nc(Cl)c([N+](=O)[O-])c(Cl)n1
Mol. weight [g/mol]: 222.03
CAS: 6237-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	2.254		Crippen Method
mcvol	133.500	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6237952&Units=SI

Legend

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

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