9H-Purine, 6-chloro-9-(methoxymethyl)-

Other names: 6-Chloro-9-methoxymethylpurine
Inchi: InChI=1S/C7H7ClN4O/c1-13-4-12-3-11-5-6(8)9-2-10-7(5)12/h2-3H,4H2,1H3
InchiKey: SZLMRHFSYVCXQX-UHFFFAOYSA-N
Formula: C7H7ClN4O
SMILES: COCn1cnc2c(Cl)ncnc21
Mol. weight [g/mol]: 198.61
CAS: 6504-64-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.084		Crippen Method
mcvol	128.600	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=C6504649&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