Caffeine, 8-chloro

Other names: 8-chloro-3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione
Inchi: InChI=1S/C8H9ClN4O2/c1-11-4-5(10-7(11)9)12(2)8(15)13(3)6(4)14/h1-3H3
InchiKey: HGKPGBJNNATDRR-UHFFFAOYSA-N
Formula: C8H9ClN4O2
SMILES: Cn1c(=O)c2c(nc(Cl)n2C)n(C)c1=O
Mol. weight [g/mol]: 228.64
CAS: 4921-49-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.44		Crippen Method
logp	-0.376		Crippen Method
mcvol	148.560	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4921497&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