

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

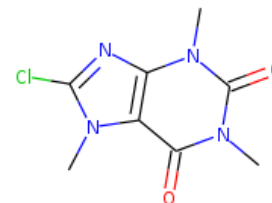
InChI Key: HGKPGBJNNATDRR-UHFFFAOYSA-N

Formula: C₈H₉ClN₄O₂

SMILES: Cn1c(Cl)nc2c1c(=O)n(C)c(=O)n2C

Molecular Weight: 228.64

CAS: 4921-49-7



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	-0.38		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H9ClN4O2/c1-11-4-5\(10-7\(11\)9\)12\(2\)8\(15\)13\(3\)6\(4\)14/h1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H9ClN4O2/c1-11-4-5(10-7(11)9)12(2)8(15)13(3)6(4)14/h1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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<https://www.cheméo.com/cid/16-863-6/Caffeine%2C%208-chloro>

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