

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

Latest version available from:

<https://www.chemeo.com/cid/16-863-6/Caffeine-8-chloro.pdf>

Generated by Cheméo on 2025-12-05 21:30:19.632185247 +0000 UTC m=+4718417.162225902.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.