

Cefmetazole

Other names: (6R,7S)-7-(2-((cyanomethyl)thio)acetamido)-7-methoxy-3-(((1-methyl-1H-tetrazol-5-yl)thio)acetyl)-15-cis-15H-17N7O5S3/c1-21-14(18-19-20-21)30-6-8-5-29-13-15(27-2,17-9(23)7-28-4)acid

Inchi: SNBUBQHDYVFSQF-HIFRSBDPSA-N

InchiKey: C15H17N7O5S3

Formula: COC1(NC(=O)CSCC#N)C(=O)N2C(C(=O)O)=C(CSc3nnnn3C)CSC21

SMILES: 471.55

Mol. weight [g/mol]:

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Cheméo Relay (1.0)
logp	-0.728		Crippen Method
mcvol	303.490	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Correlation and thermodynamic analysis of solubility of cefmetazole in 100 organic (ethanol + water) binary solvents at temperatures from 278.15 K to 303.15 K: <https://www.doi.org/10.1016/j.jct.2016.08.024>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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