

Acetazolamide tri-methyl derivative

Other names:	Acetazolamide, trimethyl deriv. Acetazolamide, trimethyl
Inchi:	InChI=1S/C7H12N4O3S2/c1-5(12)11(4)6-8-9-7(15-6)16(13,14)10(2)3/h1-4H3
InchiKey:	DCRPUDKKDYZYAB-UHFFFAOYSA-N
Formula:	C7H12N4O3S2
SMILES:	CC(=O)N(C)c1nnc(S(=O)(=O)N(C)C)s1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.53		Crippen Method
logp	-0.229		Crippen Method
mcvol	175.960	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=U137183&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

Latest version available from:

<https://www.chemeo.com/cid/64-176-6/Acetazolamide-tri-methyl-derivative.pdf>

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