

1-(o-Tolyl)biguanide

Inchi:	InChI=1S/C9H13N5/c1-6-4-2-3-5-7(6)13-9(12)14-8(10)11/h2-5H,1H3,(H6,10,11,12,13,14
InchiKey:	SQZCAOHYQSOZCE-UHFFFAOYSA-N
Formula:	C9H13N5
SMILES:	Cc1ccccc1N=C(N)N=C(N)N
Mol. weight [g/mol]:	191.24
CAS:	93-69-6

Physical Properties

Property code	Value	Unit	Source
logp	0.215		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
tf	417.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.cheméo.com/cid/100-145-9/1-o-Tolyl-biguanide.pdf>

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