6-Mercaptopurine

Inchi: InChI=1S/C5H4N4S/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)
InchiKey: GLVAUDGFNGKCSF-UHFFFAOYSA-N
Formula: C5H4N4S
SMILES: S=c1nc[nH]c2nc[nH]c12
Mol. weight [g/mol]: 152.18
CAS: 50-44-2

Physical Properties

Property code	Value	Unit	Source
logp	0.052		Crippen Method
mcvol	98.660	ml/mol	McGowan Method
tf	587.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

https://www.chemeo.com/cid/109-405-1/6-Mercaptopurine.pdf

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