

4-amino-N-(3-methoxypyrazin-2-yl)benzenesulfon

Inchi:	InChI=1S/C11H12N4O3S/c1-18-11-10(13-6-7-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H
InchiKey:	KXRZBTAEDBELFD-UHFFFAOYSA-N
Formula:	C11H12N4O3S
SMILES:	COc1nccnc1NS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	280.31
CAS:	152-47-6

Physical Properties

Property code	Value	Unit	Source
hvap	114.87	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.34		Cheméo Relay (1.0)
logp	0.868		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
tf	445.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point

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