

4-amino-N-(5,6-dimethoxypyrimidin-4-yl)benzenesulfonamide

Inchi:	InChI=1S/C12H14N4O4S/c1-19-10-11(14-7-15-12(10)20-2)16-21(17,18)9-5-3-8(13)4-6-9
InchiKey:	PJSFRIWCGOHTNF-UHFFFAOYSA-N
Formula:	C12H14N4O4S
SMILES:	COc1ncnc(NS(=O)(=O)c2ccc(N)cc2)c1OC
Mol. weight [g/mol]:	310.33
CAS:	2447-57-6

Physical Properties

Property code	Value	Unit	Source
hvap	116.74	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.22		Cheméo Relay (1.0)
logp	0.877		Crippen Method
mcvol	212.170	ml/mol	McGowan Method
tf	465.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<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):

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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