

2-Methyl-3-amino-4-methoxymethyl-5-aminomethyl

Inchi:	InChI=1S/C9H15N3O/c1-6-9(11)8(5-13-2)7(3-10)4-12-6/h4H,3,5,10-11H2,1-2H3
InchiKey:	MGESDKOHGQHZFN-UHFFFAOYSA-N
Formula:	C9H15N3O
SMILES:	COCc1c(CN)cnc(C)c1N
Mol. weight [g/mol]:	181.23
CAS:	35623-09-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	0.577		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
ss	370.25	J/molxK	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	307.10	J/molxK	298.15	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C35623097&Units=SI

Legend

cps:	Solid phase heat capacity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions

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