

Propionic acid,2-[(4-amino-1,3-dimethyl-1h-pyrazol-5-yl)thio]

Inchi:	InChI=1S/C8H11N3OS/c1-4-6-8(11(3)10-4)13-5(2)7(12)9-6/h5H,1-3H3,(H,9,12)
InchiKey:	YEMKWGPTBAAUIU-UHFFFAOYSA-N
Formula:	C8H11N3OS
SMILES:	Cc1nn(C)c2c1NC(=O)C(C)S2
Mol. weight [g/mol]:	197.26
CAS:	13568-77-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	1.161		Crippen Method
mcvol	141.120	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13568779&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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