Ethanol, 2-[(6-amino-5-nitro-4-pyrimidinyl)thio]-

Inchi: InChI=1S/C6H8N4O3S/c7-5-4(10(12)13)6(9-3-8-5)14-2-1-11/h3,11H,1-2H2,(H2,7,8,9)
InchiKey: CQPPLBXDFXKPHT-UHFFFAOYSA-N
Formula: C6H8N4O3S
SMILES: Nc1ncnc(SCCO)c1[N+](=O)[O-]
Mol. weight [g/mol]: 216.22
CAS: 116434-78-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.051		Crippen Method
mcvol	141.220	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116434787&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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