5-Amino-2-benzimidazolethiol

Other names:	5-amino-1,3-dihydro-2H-benzimidazole-2-thione
	5-amino-1,3-dihydro-2H-benzo[d]imidazole-2-thione
	5-amino-2-mercaptobenzimidazole
	5-aminobenzimidazole-2-thiol
Inchi:	InChI=1S/C7H7N3S/c8-4-1-2-5-6(3-4)10-7(11)9-5/h1-3H,8H2,(H2,9,10,11)
InchiKey:	BXDMTLVCACMNJO-UHFFFAOYSA-N
Formula:	C7H7N3S
SMILES:	Nc1ccc2[nH]c(S)nc2c1
Mol. weight [g/mol]:	165.22
CAS:	2818-66-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	0.952		Crippen Method
mcvol	116.860	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	172.00	J/mol×K	298.15	Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives:	https://www.doi.org/10.1016/j.jct.2018.03.002

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2818668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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