5-Amino-3,4-dimethyl-isoxazole

Other names:	5-Isoxazolamine, 3,4-dimethyl-
	3,4-dimethylisoxazol-5-ylamine
Inchi:	InChI=1S/C5H8N2O/c1-3-4(2)7-8-5(3)6/h6H2,1-2H3
InchiKey:	PYNDWPFZDQONDV-UHFFFAOYSA-N
Formula:	C5H8N2O
SMILES:	Cc1noc(N)c1C
Mol. weight [g/mol]:	112.13
CAS:	19947-75-2

Physical Properties

Property code	Value	Unit	Source
chs	-3028.20 ± 1.30	kJ/mol	NIST Webbook
hf	5.20 ± 2.80	kJ/mol	NIST Webbook
hfs	-82.70 ± 1.30	kJ/mol	NIST Webbook
log10ws	-5.56		Crippen Method
logp	0.874		Crippen Method
mcvol	87.680	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	88.00 ± 3.00	kJ/mol	308.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19947752&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume