

3-Isoxazolamine, 5-methyl-

Other names:	Isoxazole, 3-amino-5-methyl- 3-Amino-5-methylisoxazole 3-Methyl-5-aminoisoxazole 5-Methyl-3-aminoisoxazole 5-Methyl-3-isoxazolamine 5-methylisoxazol-3-ylamine
Inchi:	InChI=1S/C4H6N2O/c1-3-2-4(5)6-7-3/h2H,1H3,(H2,5,6)
InchiKey:	FKPXGNGUVSHWQQ-UHFFFAOYSA-N
Formula:	C4H6N2O
SMILES:	Cc1cc(N)no1
Mol. weight [g/mol]:	98.10
CAS:	1072-67-9

Physical Properties

Property code	Value	Unit	Source
chs	-2369.70 ± 0.54	kJ/mol	NIST Webbook
hf	20.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-61.84 ± 0.59	kJ/mol	NIST Webbook
log10ws	-5.08		Crippen Method
logp	0.565		Crippen Method
mcpvol	73.590	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	146.40	J/molxK	287.15	NIST Webbook
hsubt	82.00 ± 3.00	kJ/mol	293.00	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072679&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cps: Solid phase heat capacity
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

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