3-Amino-5-methylisoxazole

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

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
hvap	62.93	kJ/mol	Cheméo Relay (1.0)
logp	0.565		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
tb	492.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072679&Units=SI

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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