

5-Amino-3-methylisooxazole

Other names:	3-methylisoxazol-5-amine 5-Isoxazolamine, 3-methyl-
Inchi:	InChI=1S/C4H6N2O/c1-3-2-4(5)7-6-3/h2H,5H2,1H3
InchiKey:	FNXYWHTZDAVRTB-UHFFFAOYSA-N
Formula:	C4H6N2O
SMILES:	Cc1cc(N)on1
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
hf	20.85	kJ/mol	Cheméo Relay (1.0)
hvap	58.99	kJ/mol	Cheméo Relay (1.0)
logp	0.565		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
tb	487.88	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14678025&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):

Legend

hf:	Enthalpy of formation at standard conditions
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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