1,5-Dimethyl-2-pyrrolecarbonitrile

Other names:	1,5-dimethylpyrrole-2-carbonitrile
	1H-Pyrrol-2-carbonitrile, 1,5-dimethyl
	1H-Pyrrole-2-carbonitrile, 1,5-dimethyl-
Inchi:	InChI=1S/C7H8N2/c1-6-3-4-7(5-8)9(6)2/h3-4H,1-2H3
InchiKey:	DRXOPQFEWDRGKT-UHFFFAOYSA-N
Formula:	C7H8N2
SMILES:	Cc1ccc(C#N)n1C
Mol. weight [g/mol]:	120.15
CAS:	56341-36-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	1.205		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
ripol	1612.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	78.30	kJ/mol	298.15	Molecular energetics of pyrrolecarbonitriles and derivatives: A combined calorimetric and computational study

Sources

Molecular energetics of pyrrolecarbonitriles and derivatives: A combined calorimetric and computational study:	https://www.doi.org/10.1016/j.jct.2011.12.019
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56341367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices