

2-Thiophenecarbonitrile

Other names:	2-Thenylcyanide 2-cyanothiophene Thiophene-2-carbonitrile
Inchi:	InChI=1S/C5H3NS/c6-4-5-2-1-3-7-5/h1-3H
InchiKey:	CUPOOAWTRIURFT-UHFFFAOYSA-N
Formula:	C5H3NS
SMILES:	N#Cc1cccs1
Mol. weight [g/mol]:	109.15
CAS:	1003-31-2

Physical Properties

Property code	Value	Unit	Source
hvap	49.50 ± 1.10	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.83 ± 0.05	eV	NIST Webbook
log10ws	-1.58		Crippen Method
logp	1.620		Crippen Method
mcvol	79.580	ml/mol	McGowan Method
tb	465.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	49.50	kJ/mol	298.15	Thermochemistry of substituted thiophenecarbonitrile derivatives

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of substituted thiophenecarbonitrile derivatives:	https://www.doi.org/10.1016/j.jct.2007.06.020

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003312&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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