3-Thiophenecarbonitrile

Other names: Thiophene-3-carbonitrile
Inchi: InChI=1S/C5H3NS/c6-3-5-1-2-7-4-5/h1-2,4H
InchiKey: GSXCEVHRIVLFJV-UHFFFAOYSA-N
Formula: C5H3NS
SMILES: N#Cc1ccsc1
Mol. weight [g/mol]: 109.15
CAS: 1641-09-4

Physical Properties

Property code	Value	Unit	Source
hvap	51.60 ± 1.90	kJ/mol	NIST Webbook
log10ws	-1.58		Crippen Method
logp	1.620		Crippen Method
mcvol	79.580	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	51.60	kJ/mol	298.15	Thermochemistry of substituted thiophenecarbonitrile derivatives

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1641094&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
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