3-Methylthiophene-2-carbonitrile

Other names: 3-Methyl-2-thiophenecarbonitrile
Inchi: InChI=1S/C6H5NS/c1-5-2-3-8-6(5)4-7/h2-3H,1H3
InchiKey: ALZHYEITUZEZMT-UHFFFAOYSA-N
Formula: C6H5NS
SMILES: Cc1ccsc1C#N
Mol. weight [g/mol]: 123.18
CAS: 55406-13-8

Physical Properties

Property code	Value	Unit	Source
hvap	54.40 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.928		Crippen Method
mcvol	93.670	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	54.40	kJ/mol	298.15	Thermochemistry of substituted thiophenecarbonitrile derivatives

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55406138&Units=SI
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

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

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