

# 2-Thiopheneacetonitrile

<b>Other names:</b>	2-(Cyanomethyl)thiophene 2-Thienylacetonitrile Thiophene-2-acetonitrile
<b>Inchi:</b>	InChI=1S/C6H5NS/c7-4-3-6-2-1-5-8-6/h1-2,5H,3H2
<b>InchiKey:</b>	CLSHQIDDCJTHAJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H5NS
<b>SMILES:</b>	N#CCc1cccs1
<b>Mol. weight [g/mol]:</b>	123.18
<b>CAS:</b>	20893-30-5

## Physical Properties

Property code	Value	Unit	Source
hvap	60.50 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.814		Crippen Method
mvol	93.670	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.50	kJ/mol	298.15	Thermochemistry of substituted thiophenecarbonitrile derivatives

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	2.90	NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20893305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20893305&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Thermochemistry of substituted thiophenecarbonitrile derivatives:</b>	<a href="https://www.doi.org/10.1016/j.jct.2007.06.020">https://www.doi.org/10.1016/j.jct.2007.06.020</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>h<sub>vapt</sub>:</b>	Enthalpy of vaporization at a given temperature
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>t<sub>brp</sub>:</b>	Boiling point at reduced pressure

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