3-Thiopheneacetonitrile

Other names:	3-thienylacetonitrile
	Thiophene-3-acetonitrile
Inchi:	InChI=1S/C6H5NS/c7-3-1-6-2-4-8-5-6/h2,4-5H,1H2
InchiKey:	GWZCLMWEJWPFFA-UHFFFAOYSA-N
Formula:	C6H5NS
SMILES:	N#CCc1ccsc1
Mol. weight [g/mol]:	123.18
CAS:	13781-53-8

Physical Properties

Property code	Value	Unit	Source
hvap	61.10 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.814		Crippen Method
mcvol	93.670	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	61.10	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=C13781538&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