2-Thiophenemethanamine

Other names:	2-Aminomethylthiophene
	2-Thenylamine
	2-Thienylmethylamine
	2-Thiophenemethylamine
	Thiophene-2-methylamine
	2-(2-Aminomethyl)thiophene
Inchi:	InChI=1S/C5H7NS/c6-4-5-2-1-3-7-5/h1-3H,4,6H2
InchiKey:	FKKJJPMGAWGYPN-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	NCc1cccs1
Mol. weight [g/mol]:	113.18
CAS:	27757-85-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	1.207		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
ripol	1963.00		NIST Webbook
ripol	1963.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.20	K	3.70	NIST Webbook
tbrp	348.00	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27757853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure