

2-Furanmethanamine

Other names:	Furfurylamine
	«alpha»-Furfurylamine
	2-(Aminomethyl)furan
	2-Furanmethylaniline
	2-Furfurylamine
	Methylaniline, 1-(2-furyl)-
	USAF Q-1
	(2-Furylmethyl)amine
	UN 2526
	(2-Furanylmethyl)amine
	NSC 49136
	NSC 61168
	InChI=1S/C5H7NO/c6-4-5-2-1-3-7-5/h1-3H,4,6H2
Inchi:	
InchiKey:	DDRPCXLAQZKBJP-UHFFFAOYSA-N
Formula:	C5H7NO
SMILES:	NCc1ccco1
Mol. weight [g/mol]:	97.12
CAS:	617-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	0.738		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
rinpol	854.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	854.00		NIST Webbook
tb	418.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	11.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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