

2-Furancarbonitrile

Other names:	2-Furonitrile «alpha»-Furyl cyanide 2-Cyanofuran 2-Furyl cyanide Furan-2-carbonitrile
Inchi:	InChI=1S/C5H3NO/c6-4-5-2-1-3-7-5/h1-3H
InchiKey:	YXDXXGXWFJCXEB-UHFFFAOYSA-N
Formula:	C5H3NO
SMILES:	N#Cc1ccco1
Mol. weight [g/mol]:	93.08
CAS:	617-90-3

Physical Properties

Property code	Value	Unit	Source
hvap	44.80 ± 0.40	kJ/mol	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
ie	9.47 ± 0.05	eV	NIST Webbook
log10ws	-5.56		Crippen Method
logp	1.151		Crippen Method
mvol	69.100	ml/mol	McGowan Method
rinpol	776.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	822.00		NIST Webbook
tb	420.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	98.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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