Cyanopyrazine

Other names:	2-Cyanopyrazine
	2-Pyrazinecarbonitrile
	Pyrazine-2-carbonitrile
	Pyrazinecarbonitrile-
	Pyrazinenitrile
	Pyrazinonitrile
Inchi:	InChI=1S/C5H3N3/c6-3-5-4-7-1-2-8-5/h1-2,4H
InchiKey:	PMSVVUSIPKHUMT-UHFFFAOYSA-N
Formula:	C5H3N3
SMILES:	N#Cc1cnccn1
Mol. weight [g/mol]:	105.10
CAS:	19847-12-2

Physical Properties

Property code	Value	Unit	Source
hvap	58.70 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	0.348		Crippen Method
mcvol	78.890	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rfi	1.53400		293.15	Activity coefficients in binary mixtures formed by cyclohexanone with a variety of compounds at 94.7 kPa

rfi	1.53400		293.15	(Vapor + liquid) equilibrium of binary mixtures formed by N,N-dimethyl formamide with some compounds at 95.1 kPa

Sources

Activity coefficients in binary mixtures formed by cyclohexanone with a variety of compounds at 94.7 kPa:	https://www.doi.org/10.1016/j.fluid.2005.06.022
(Vapor + liquid) equilibrium of binary mixtures formed by N,N-dimethyl formamide with some compounds at 95.1 kPa:	https://www.doi.org/10.1016/j.fluid.2007.02.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19847122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rfi:	Refractive Index