3-Methylpyridazine

Other names: Pyridazine, 3-methyl-
Inchi: InChI=1S/C5H6N2/c1-5-3-2-4-6-7-5/h2-4H,1H3
InchiKey: MXDRPNGTQDRKQM-UHFFFAOYSA-N
Formula: C5H6N2
SMILES: Cc1cccnn1
Mol. weight [g/mol]: 94.11
CAS: 1632-76-4

Physical Properties

Property code	Value	Unit	Source
hvap	49.70 ± 2.80	kJ/mol	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.785		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	969.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	487.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	58.00	kJ/mol	298.15	Vaporization, Sublimation Enthalpy, and Crystal Structures of Imidazo[1,2-a]pyrazine and Phthalazine

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1632764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization, Sublimation Enthalpy, and Crystal Structures of Imidazo[1,2-a]pyrazine and Phthalazine:	https://www.doi.org/10.1021/acs.jced.5b00606
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature