Pyrazine, methyl-

Other names:	2-Methylpyrazine
	2-methyl-1,4-diazine
	Methylpyrazine
	Pyrazine, 2-methyl-
Inchi:	InChI=1S/C5H6N2/c1-5-4-6-2-3-7-5/h2-4H,1H3
InchiKey:	CAWHJQAVHZEVTJ-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	Cc1cnccn1
Mol. weight [g/mol]:	94.11
CAS:	109-08-0

Physical Properties

Property code	Value	Unit	Source
hvap	43.70 ± 1.90	kJ/mol	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.785		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpol	802.80		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	812.00		NIST Webbook
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ripol	1235.00		NIST Webbook
tb	408.85 ± 0.30	K	NIST Webbook

tb	409.15 ± 1.50	K	NIST Webbook
tb	405.15 ± 1.50	K	NIST Webbook
tf	244.35 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	42.40	kJ/mol	340.00	NIST Webbook
pvap	4.48	kPa	323.13	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions
pvap	0.46	kPa	283.27	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions
pvap	0.87	kPa	293.24	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions
pvap	1.56	kPa	303.18	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions

pvap	2.70	kPa	313.12	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	
pvap	0.23	kPa	273.47	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	
pvap	7.15	kPa	333.11	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	
pvap	11.03	kPa	343.05	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	
pvap	16.61	kPa	353.03	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	
pvap	24.08	kPa	362.95	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions	

pvap	0.11	kPa	263.72	Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions
rfi	1.50500		293.15	Activity coefficients in binary mixtures formed by cyclohexanone with a variety of compounds at 94.7 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	101.00	NIST Webbook

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1343.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Isothermal vapor-liquid equilibria and excess molar enthalpy of 2-methylpyrazine (2MP) containing binary mixtures. Comparison with DISQUAC predictions:	https://www.doi.org/10.1016/j.fluid.2015.03.033
Solubility of Pyrazine and its Derivatives in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je0601457

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
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point