

Pyrazine, tetramethyl-

Other names:	2,3,5,6-Tetramethylpyrazine BS Factor Pyrazine, 2,3,5,6-tetramethyl Tetramethylpyrazin ligustrazine tetramethylpyrazine tetrapyrazine
Inchi:	InChI=1S/C8H12N2/c1-5-6(2)10-8(4)7(3)9-5/h1-4H3
InchiKey:	FINHMKGKINIASC-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	Cc1nc(C)c(C)nc1C
Mol. weight [g/mol]:	136.19
CAS:	1124-11-4

Physical Properties

Property code	Value	Unit	Source
chs	-4823.20 ± 1.70	kJ/mol	NIST Webbook
hf	54.70 ± 4.50	kJ/mol	NIST Webbook
hfs	-39.90 ± 2.00	kJ/mol	NIST Webbook
hsub	94.60 ± 4.00	kJ/mol	NIST Webbook
hsub	94.60 ± 4.00	kJ/mol	NIST Webbook
hsub	94.60	kJ/mol	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	1.710		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1096.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.68		NIST Webbook

rinpol	1105.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1062.20	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1065.60	NIST Webbook
rinpol	1069.30	NIST Webbook
rinpol	1062.90	NIST Webbook
rinpol	1096.00	NIST Webbook
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ripol	1453.00	NIST Webbook
ripol	1439.00	NIST Webbook

ripol	1468.00		NIST Webbook
tb	463.20	K	NIST Webbook
tf	358.50 ± 0.30	K	NIST Webbook
tf	358.55	K	Measurement and Correlation of the Solubility of Tetramethylpyrazine in Nine Monosolvents and Two Binary Solvent Systems

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of the Solubility of Tetramethylpyrazine in Nine Monosolvents and Two Binary Solvent Systems	https://www.doi.org/10.1021/acs.jced.8b00888
Tetramethylpyrazine in Supercritical Carbon Dioxide	https://www.doi.org/10.1021/je049715y
McGowan's Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124114&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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