

Pyrazine, trimethyl-

Other names:	Trimethylpyrazine 2,3,5-Trimethylpyrazine 2,3,6-Trimethylpyrazine Pyrazine, 2,3,5-trimethyl
Inchi:	InChI=1S/C7H10N2/c1-5-4-8-6(2)7(3)9-5/h4H,1-3H3
InchiKey:	IAEGWXHKWJGQAZ-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	Cc1cnc(C)c(C)n1
Mol. weight [g/mol]:	122.17
CAS:	14667-55-1

Physical Properties

Property code	Value	Unit	Source
chl	-4204.10 ± 2.00	kJ/mol	NIST Webbook
hf	74.30 ± 2.70	kJ/mol	NIST Webbook
hfl	20.40 ± 2.20	kJ/mol	NIST Webbook
hvap	53.90 ± 1.60	kJ/mol	NIST Webbook
hvap	53.90 ± 1.60	kJ/mol	NIST Webbook
hvap	53.90	kJ/mol	NIST Webbook
log10ws	-2.43		Crippen Method
logp	1.402		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	1001.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1004.00		NIST Webbook
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Sources

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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=C14667551&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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