

Pyrazine, 2,5-dimethyl-

Other names:	2,5-Dimethylpyrazine
Inchi:	InChI=1S/C6H8N2/c1-5-3-8-6(2)4-7-5/h3-4H,1-2H3
InchiKey:	LCZUOKDVTBMCXM-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	Cc1cnc(C)cn1
Mol. weight [g/mol]:	108.14
CAS:	123-32-0

Physical Properties

Property code	Value	Unit	Source
hvap	47.20 ± 2.20	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	892.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	930.00		NIST Webbook
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rinpol	890.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	913.00		NIST Webbook
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rinpol	891.00	NIST Webbook
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ripol	1338.00		NIST Webbook
tb	428.15 ± 2.00	K	NIST Webbook

tb	427.25 ± 1.50	K	NIST Webbook
tb	428.20	K	NIST Webbook
tf	257.65 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	44.50	kJ/mol	357.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
tf:	Normal melting (fusion) point

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