

# Pyrazine

<b>Other names:</b>	1,4-DIAZABENZENE 1,4-Diazine P-DIAZINE PARADIAZINE Piazine para-diazine
<b>Inchi:</b>	InChI=1S/C4H4N2/c1-2-6-4-3-5-1/h1-4H
<b>InchiKey:</b>	KYQCOXFCLRTKLS-UHFFFAOYSA-N
<b>Formula:</b>	C4H4N2
<b>SMILES:</b>	c1cnccn1
<b>Mol. weight [g/mol]:</b>	80.09
<b>CAS:</b>	290-37-9

## Physical Properties

Property code	Value	Unit	Source
af	0.2400		KDB
affp	877.10	kJ/mol	NIST Webbook
basg	847.00	kJ/mol	NIST Webbook
chl	-2285.50 ± 1.20	kJ/mol	NIST Webbook
ea	-0.07	eV	NIST Webbook
hf	196.10 ± 1.50	kJ/mol	NIST Webbook
hfl	139.80 ± 1.20	kJ/mol	NIST Webbook
hvap	56.27 ± 0.46	kJ/mol	NIST Webbook
hvap	56.30	kJ/mol	NIST Webbook
hvap	40.50 ± 1.70	kJ/mol	NIST Webbook
ie	9.28 ± 0.05	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.29 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.28 ± 0.01	eV	NIST Webbook
ie	9.29	eV	NIST Webbook
ie	9.29 ± 0.03	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
log10ws	-1.00		Crippen Method
logp	0.477		Crippen Method

mcvol	63.420	ml/mol	McGowan Method
pc	5800.00	kPa	KDB
rinpol	731.60		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	708.00		NIST Webbook
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rinpol	706.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	732.00		NIST Webbook
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rinpol	710.00		NIST Webbook
rinpol	706.00		NIST Webbook

rinpol	722.00	NIST Webbook
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rinpol	718.00	NIST Webbook
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rinpol	734.00	NIST Webbook
rinpol	740.00	NIST Webbook
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rinpol	745.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	744.00	NIST Webbook

ripol	740.00	NIST Webbook
ripol	738.00	NIST Webbook
ripol	730.00	NIST Webbook
ripol	1204.00	NIST Webbook
ripol	1209.00	NIST Webbook
ripol	1179.00	NIST Webbook
ripol	1207.00	NIST Webbook
ripol	1210.00	NIST Webbook
ripol	1201.00	NIST Webbook
ripol	1216.00	NIST Webbook
ripol	1196.00	NIST Webbook
ripol	1194.00	NIST Webbook
ripol	1179.00	NIST Webbook
ripol	1224.00	NIST Webbook
ripol	1218.00	NIST Webbook
ripol	1194.00	NIST Webbook
ripol	1222.00	NIST Webbook
ripol	1196.00	NIST Webbook
ripol	1214.00	NIST Webbook
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ripol	1201.00	NIST Webbook
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ripol	1204.00		NIST Webbook
ripol	1206.00		NIST Webbook
ripol	1219.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1228.00		NIST Webbook
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ripol	1243.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1232.00		NIST Webbook
tb	390.35 ± 0.50	K	NIST Webbook
tb	388.65 ± 1.00	K	NIST Webbook
tb	388.70	K	NIST Webbook
tb	388.60	K	KDB
tc	622.00	K	KDB
tf	334.05 ± 6.00	K	NIST Webbook
tf	320.15 ± 1.00	K	NIST Webbook
tf	324.00 ± 0.10	K	NIST Webbook
tf	326.00	K	KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	180.00	J/molxK	298.00	NIST Webbook
hfust	14.78	kJ/mol	192.50	NIST Webbook
hfust	12.95	kJ/mol	328.20	NIST Webbook
hsubt	56.20	kJ/mol	302.50	NIST Webbook
hvapt	38.80 ± 0.10	kJ/mol	390.00	NIST Webbook
hvapt	36.50 ± 0.20	kJ/mol	390.00	NIST Webbook
hvapt	34.10 ± 0.40	kJ/mol	390.00	NIST Webbook
hvapt	37.90	kJ/mol	352.50	NIST Webbook

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	102.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Solubility of Pyrazine and Its Derivatives in Supercritical Carbon Dioxide:</b>	<a href="https://www.doi.org/10.1021/je0601457">https://www.doi.org/10.1021/je0601457</a>
<b>McGowan Method:</b>	<a href="https://www.cheric.org/files/research/kdb/mol/mol1337.mol">https://www.cheric.org/files/research/kdb/mol/mol1337.mol</a>
<b>NIST Webbook:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C290379&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C290379&amp;Units=SI</a>
	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>af:</b>	Acentric Factor
<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cps:</b>	Solid phase heat capacity
<b>ea:</b>	Electron affinity
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices

<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

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