Pyrazine, 2,3-dimethyl-

Other names: 2,3-Dimethylpyrazine
Inchi: InChI=1S/C6H8N2/c1-5-6(2)8-4-3-7-5/h3-4H,1-2H3
InchiKey: OXQOBQJCDNLAPO-UHFFFAOYSA-N
Formula: C6H8N2
SMILES: Cc1nccnc1C
Mol. weight [g/mol]: 108.14
CAS: 5910-89-4

Physical Properties

Property code	Value	Unit	Source
chl	-3577.80 ± 1.70	kJ/mol	NIST Webbook
hf	126.00	kJ/mol	NIST Webbook
hfl	73.40 ± 2.00	kJ/mol	NIST Webbook
hvap	52.60	kJ/mol	NIST Webbook
hvap	52.60 ± 1.70	kJ/mol	NIST Webbook
hvap	52.60	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	927.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	900.00		NIST Webbook
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Sources

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NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5910894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Pyrazine and Its Derivatives in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je0601457

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