3,5-Dimethylpyrazole

Other names:	1(H)-3,5-Dimethylpyrazole
	1H-Pyrazole, 3,5-dimethyl-
	3,5 DMP
	3,5-Dimethyl-1H-pyrazole
	3,5-Dwumetylopirazolu
	NSC 8729
	Pyrazole, 3,5-dimethyl-
	TH 564
	U 6245
Inchi:	InChI=1S/C5H8N2/c1-4-3-5(2)7-6-4/h3H,1-2H3,(H,6,7)
InchiKey:	SDXAWLJRERMRKF-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1cc(C)[nH]n1
Mol. weight [g/mol]:	96.13
CAS:	67-51-6

Physical Properties

Property code	Value	Unit	Source
affp	933.50	kJ/mol	NIST Webbook
basg	900.10	kJ/mol	NIST Webbook
hsub	83.40 ± 2.40	kJ/mol	NIST Webbook
ie	8.75 ± 0.03	eV	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.545		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	1010.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1010.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1675.00		NIST Webbook
tb	491.20	K	NIST Webbook

tf	381.75	K	Solubility determination and thermodynamic modelling of 3,5-dimethylpyrazole in nine organic solvents from T = (283.15 to 313.15) K and mixing properties of solutions

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	83.30 ± 0.20	kJ/mol	301.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility determination and thermodynamic modelling of 3,5-dimethylpyrazole in nine organic solvents from T = (283.15 to 313.15) K and mixing properties of solutions:	https://www.doi.org/10.1016/j.jct.2017.02.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
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