

2,3-Pyrazinedicarbonitrile

Other names:	2,3-Dicyanopyrazine
Inchi:	InChI=1S/C6H2N4/c7-3-5-6(4-8)10-2-1-9-5/h1-2H
InchiKey:	OTVZGAXESBAAQQ-UHFFFAOYSA-N
Formula:	C6H2N4
SMILES:	N#Cc1nccnc1C#N
Mol. weight [g/mol]:	130.11
CAS:	13481-25-9

Physical Properties

Property code	Value	Unit	Source
hfus	19.80	kJ/mol	Thermochemical study of cyanopyrazines: Experimental and theoretical approaches
hsub	89.10 ± 2.70	kJ/mol	NIST Webbook
log10ws	-1.71		Crippen Method
logp	0.220		Crippen Method
mcvol	94.360	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.80	kJ/mol	405.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13481259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study of cyanopyrazines: Experimental and theoretical approaches:	https://www.doi.org/10.1016/j.jct.2005.07.006
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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