1H-Imidazole, 2-ethyl-

Other names:	2-ethyl-1H-imidazole
	2-ethylimidazole
	imidazole, 2-ethyl-
Inchi:	InChI=1S/C5H8N2/c1-2-5-6-3-4-7-5/h3-4H,2H2,1H3,(H,6,7)
InchiKey:	PQAMFDRRWURCFQ-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	CCc1ncc[nH]1
Mol. weight [g/mol]:	96.13
CAS:	1072-62-4

Physical Properties

Property code	Value	Unit	Source
chs	-3089.60 ± 1.00	kJ/mol	NIST Webbook
hf	68.30 ± 1.30	kJ/mol	NIST Webbook
hfs	-21.30 ± 1.20	kJ/mol	NIST Webbook
hsub	89.60 ± 0.40	kJ/mol	NIST Webbook
hsub	89.60	kJ/mol	NIST Webbook
hsub	89.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.26		Crippen Method
logp	0.490		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
tb	541.20	K	NIST Webbook
tt	282.00	K	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	147.08	J/mol×K	298.15	NIST Webbook
hsubt	89.20 ± 0.40	kJ/mol	312.00	NIST Webbook

Sources

Heat capacities and thermodynamic functions of the ZIF organic linkers Imidazole, 2-methylimidazole, and 2-ethylimidazole:	https://www.doi.org/10.1016/j.jct.2018.12.024
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tt:	Triple Point Temperature