

1H-Pyrrole-2-carboxylic acid

Other names:	Pyrrole-2-carboxylic acid Minalin Minaline PCA
Inchi:	InChI=1S/C5H5NO2/c7-5(8)4-2-1-3-6-4/h1-3,6H,(H,7,8)
InchiKey:	WRHZVMBBRYBTKZ-UHFFFAOYSA-N
Formula:	C5H5NO2
SMILES:	O=C(O)c1ccc[nH]1
Mol. weight [g/mol]:	111.10
CAS:	634-97-9

Physical Properties

Property code	Value	Unit	Source
hsub	100.80 ± 0.90	kJ/mol	NIST Webbook
log10ws	-0.75		Crippen Method
logp	0.231		Crippen Method
mcvol	79.270	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	98.60 ± 0.90	kJ/mol	342.00	NIST Webbook
hsubt	126.80	kJ/mol	352.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C634979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/40-148-3/1H-Pyrrole-2-carboxylic-acid.pdf>

Generated by Cheméo on 2025-12-06 00:51:20.041585951 +0000 UTC m=+4730477.571626616.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.