N-Methylpyrrole-2-carboxylic acid

Other names:	1H-Pyrrole-2-carboxylic acid, 1-methyl- 1-Methyl-2-pyrrolecarboxylic acid
Inchi:	InChI=1S/C6H7NO2/c1-7-4-2-3-5(7)6(8)9/h2-4H,1H3,(H,8,9)
InchiKey:	ILAOVOOZLVGAJF-UHFFFAOYSA-N
Formula:	C6H7NO2
SMILES:	Cn1cccc1C(=O)O
Mol. weight [g/mol]:	125.13
CAS:	6973-60-0

Physical Properties

Property code	Value	Unit	Source
hsub	96.20 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.82		Crippen Method
logp	0.723		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	95.30 ± 0.70	kJ/mol	316.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C6973600&Units=SI

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