

# 3-Furancarboxylic acid

Other names:	3-Furoic acid
Inchi:	InChI=1S/C5H4O3/c6-5(7)4-1-2-8-3-4/h1-3H,(H,6,7)
InchiKey:	IHCCAYCGZOLTEU-UHFFFAOYSA-N
Formula:	C5H4O3
SMILES:	O=C(O)c1ccoc1
Mol. weight [g/mol]:	112.08
CAS:	488-93-7

## Physical Properties

Property code	Value	Unit	Source
hsub	87.10 ± 0.50	kJ/mol	NIST Webbook
log10ws	-5.27		Crippen Method
logp	0.978		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.30	kJ/mol	394.80	NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C488937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C488937&amp;Units=SI</a>

# Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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