3-Furaldehyde

Other names:	3-Furancarboxaldehyde
	3-Formylfuran
	3-Furancarbaldehyde
	3-Furfural
	Furan-3-carboxaldehyde
Inchi:	InChI=1S/C5H4O2/c6-3-5-1-2-7-4-5/h1-4H
InchiKey:	AZVSIHIBYRHSLB-UHFFFAOYSA-N
Formula:	C5H4O2
SMILES:	O=Cc1ccoc1
Mol. weight [g/mol]:	96.08
CAS:	498-60-2

Physical Properties

Property code	Value	Unit	Source
hvap	48.10 ± 0.50	kJ/mol	NIST Webbook
log10ws	-5.45		Crippen Method
logp	1.092		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
rinpol	833.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	831.70		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	846.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1454.00		NIST Webbook

ripol	1448.00	NIST Webbook
ripol	1437.00	NIST Webbook
ripol	1426.00	NIST Webbook
ripol	1483.00	NIST Webbook
ripol	1454.00	NIST Webbook
ripol	1458.00	NIST Webbook
ripol	1455.00	NIST Webbook
ripol	1455.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	97.60	NIST Webbook
tbrp	344.20	K	5.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C498602&Units=SI
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

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tbrp: Boiling point at reduced pressure

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