

3-Thiophenecarboxaldehyde

Other names:	3-Formylthiophene Thiophene-3-aldehyde Thiophene-3-carboxaldehyde 3-Thiophenaldehyde 3-Thienophenecarboxyaldehyde 3-Carboxaldehyde-thiophene 3-Thiophene carboxyaldehyde Thiophen-3-carboxaldehyde thiophene-3-carbaldehyde
Inchi:	InChI=1S/C5H4OS/c6-3-5-1-2-7-4-5/h1-4H
InchiKey:	RBIGKSZIQCTIJF-UHFFFAOYSA-N
Formula:	C5H4OS
SMILES:	O=Cc1ccsc1
Mol. weight [g/mol]:	112.15
CAS:	498-62-4

Physical Properties

Property code	Value	Unit	Source
hvap	52.60 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.561		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
rinpol	960.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	974.00		NIST Webbook

ripol	957.00	NIST Webbook
ripol	952.00	NIST Webbook
ripol	952.00	NIST Webbook
ripol	1003.00	NIST Webbook
ripol	1003.00	NIST Webbook
ripol	960.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1693.00	NIST Webbook
ripol	1684.00	NIST Webbook
ripol	1657.00	NIST Webbook
ripol	1678.00	NIST Webbook
ripol	1685.00	NIST Webbook
ripol	1687.00	NIST Webbook
ripol	1693.00	NIST Webbook
ripol	1684.00	NIST Webbook
ripol	1678.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1687.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1687.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.90	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C498624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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