2-Thiophenecarboxaldehyde

Other names:	2-Carboxaldehyde-thiophene
	2-Formylthiophene
	2-Thienaldehyde
	2-Thienylaldehyde
	2-Thienylcarboxaldehyde
	2-Thiophenaldehyde
	2-Thiophencarboxaldehyde
	2-Thiophene carboxyaldehyde
	2-Thiophenecarbaldehyde
	2-thiophenealdehyde
	2-thiophenic aldehyde
	NSC 2162
	Thiophene-2-aldehyde
	Thiophene-2-carbaldehyde
	Thiophene-2-carboxaldehyde
	thiophen-2-carboxaldehyde
	thiophenecarboxaldehyde
	«alpha»-Formylthiophene
	«alpha»-Thiophenecarboxaldehyde
Inchi:	InChI=1S/C5H4OS/c6-4-5-2-1-3-7-5/h1-4H
InchiKey:	CNUDBTRUORMMPA-UHFFFAOYSA-N
Formula:	C5H4OS
SMILES:	O=Cc1cccs1
Mol. weight [g/mol]:	112.15
CAS:	98-03-3

Physical Properties

Property code	Value	Unit	Source
hvap	54.90 ± 1.10	kJ/mol	NIST Webbook
ie	9.37 ± 0.05	eV	NIST Webbook
ie	9.55 ± 0.05	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.561		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1010.00		NIST Webbook

rinpol	962.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1004.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	995.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1026.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	987.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	965.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	971.00	NIST Webbook
rinpol	990.00	NIST Webbook
rinpol	974.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	990.00	NIST Webbook
rinpol	974.00	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	962.00	NIST Webbook
ripol	1714.00	NIST Webbook
ripol	1684.00	NIST Webbook
ripol	1655.00	NIST Webbook

ripol	1702.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	470.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	0.66	kPa	336.42	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

pvap	0.85	kPa	340.70	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	1.14	kPa	345.63	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	1.40	kPa	349.65	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	1.73	kPa	353.70	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	1.92	kPa	356.19	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	2.27	kPa	359.55	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	2.55	kPa	361.67	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	2.92	kPa	364.68	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	3.27	kPa	366.94	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	3.60	kPa	368.98	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	4.14	kPa	372.07	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	4.64	kPa	374.68	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	5.07	kPa	376.79	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	5.30	kPa	377.74	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	5.80	kPa	379.92	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	6.50	kPa	382.69	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	7.58	kPa	386.72	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	8.41	kPa	389.41	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	9.29	kPa	391.94	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	10.41	kPa	394.82	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	12.29	kPa	399.42	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	13.11	kPa	401.02	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	14.06	kPa	403.00	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	15.05	kPa	404.90	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	16.14	kPa	407.06	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	17.25	kPa	408.95	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	18.60	kPa	411.16	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	19.66	kPa	412.82	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

pvap	20.41	kPa	413.90	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	21.80	kPa	415.91	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	23.36	kPa	418.01	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	24.95	kPa	420.05	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	26.60	kPa	422.07	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	28.25	kPa	424.04	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	
pvap	30.11	kPa	426.15	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling	

pvap	32.01	kPa	428.14	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	32.92	kPa	429.02	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	34.05	kPa	430.17	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	35.47	kPa	431.54	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling
pvap	37.20	kPa	433.17	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling

Sources

Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling:	https://www.doi.org/10.1016/j.jct.2017.07.008
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature