

Ethanone, 1-(3-thienyl)-

Other names:	3-acetylthiophene Ketone, methyl 3-thienyl methyl 3-thienyl ketone
Inchi:	InChI=1S/C6H6OS/c1-5(7)6-2-3-8-4-6/h2-4H,1H3
InchiKey:	RNIDWJDZNNVFDY-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	CC(=O)c1ccsc1
Mol. weight [g/mol]:	126.18
CAS:	1468-83-3

Physical Properties

Property code	Value	Unit	Source
hfus	18.90	kJ/mol	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
ie	9.32 ± 0.05	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.951		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1731.00		NIST Webbook
tf	334.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.90	kJ/mol	333.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	482.20	K	99.70	NIST Webbook
tbrp	351.50 ± 0.50	K	0.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of sulfur heterocycles: Thiane and thiophene	https://www.doi.org/10.1016/j.tca.2005.11.024
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1468833&Units=SI

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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