

2(5H)-Thiophenone

Other names:	2-Butenoic acid, 4-mercapto-, «gamma»-(thio lactone) 2,5-Dihydrothiophenone
Inchi:	InChI=1S/C4H4OS/c5-4-2-1-3-6-4/h1-2H,3H2
InchiKey:	NMSLUAZZTFUUFZ-UHFFFAOYSA-N
Formula:	C4H4OS
SMILES:	O=C1C=CCS1
Mol. weight [g/mol]:	100.14
CAS:	3354-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-25.71	kJ/mol	Joback Method
hf	-79.73	kJ/mol	Joback Method
hfus	3.37	kJ/mol	Joback Method
hvap	56.00 ± 1.20	kJ/mol	NIST Webbook
ie	9.78 ± 0.05	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	0.816		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
pc	5704.58	kPa	Joback Method
tb	425.68	K	Joback Method
tc	669.83	K	Joback Method
tf	302.41	K	Joback Method
vc	0.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.44	J/mol×K	425.68	Joback Method
cpg	124.02	J/mol×K	466.37	Joback Method
cpg	132.16	J/mol×K	507.06	Joback Method
cpg	139.87	J/mol×K	547.76	Joback Method
cpg	147.14	J/mol×K	588.45	Joback Method
cpg	153.97	J/mol×K	629.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	1.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3354323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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