

Dihydro-3-(2H)-thiophenone

Other names:	3(2H)-Thiophenone, dihydro- 3-Oxo-2,3,4,5-tetrahydrothiophene 3-Oxotetrahydrothiophene 3-Thiacyclopentanone 3-Thiophanone 4,5-Dihydro-3(2H)-thiophenone NSC 241151 Tetrahydrothiophen-3-one Tetrahydrothiophene-3-one Thiolan-3-one dihydro-3-(2H)-thiophenone (tetrahydrothiophen-3-one) dihydrothiophen-3(2H)-one
Inchi:	InChI=1S/C4H6OS/c5-4-1-2-6-3-4/h1-3H2
InchiKey:	DSXFPRKPFJRPIB-UHFFFAOYSA-N
Formula:	C4H6OS
SMILES:	O=C1CCSC1
Mol. weight [g/mol]:	102.16
CAS:	1003-04-9

Physical Properties

Property code	Value	Unit	Source
chl	-2848.00 ± 1.70	kJ/mol	NIST Webbook
gf	-55.67	kJ/mol	Joback Method
hf	-135.30 ± 2.00	kJ/mol	NIST Webbook
hfus	2.15	kJ/mol	Joback Method
hvap	50.10 ± 0.80	kJ/mol	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.692		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
rinpol	906.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	916.00		NIST Webbook

rinpol	913.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	959.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	448.20	K	NIST Webbook
tc	667.95	K	Joback Method
tf	301.65	K	Joback Method
vc	0.255	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.08	J/mol×K	426.52	Joback Method
cpg	139.26	J/mol×K	466.76	Joback Method
cpg	148.95	J/mol×K	507.00	Joback Method
cpg	158.14	J/mol×K	547.23	Joback Method
cpg	166.85	J/mol×K	587.47	Joback Method
cpg	175.06	J/mol×K	627.71	Joback Method

cpg	182.78	J/mol×K	667.95	Joback Method
-----	--------	---------	--------	---------------

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.50 ± 1.50	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.76415e+01
Coeff. B	-5.83698e+03
Temperature range (K), min.	336.35
Temperature range (K), max.	473.40

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1003049&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/49-172-7/Dihydro-3-2H-thiophenone.pdf>

Generated by Cheméo on 2025-12-06 01:48:33.140814 +0000 UTC m=+4733910.670854654.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.