2-METHYLTETRAHYDROTHIOPHEN-3-ONE

Other names:	Dihydro-2-methyl-3(2H)-thiophenone
	2-Methyltetrahydrothiophen-3-one
	2-Methyldihydro-3(2H)-thiophenone
	2-Methyl-3-thiolanone
	2-methyl-4,5-dihydro-3(2H)-thiophenone
	2-Methyltetrahydrothiophene-3-one
	2-Methylthiolan-3-one
	2-Methytetrahydrothiophen-3-one
	4,5-Dihydro-2-methyl-3(2H)-thiophenone
	4,5-Dihydro-2-methylthiophen-3(2H)-one
	Dihydro-3(2H)-thiophenone, 2-methyl
	Thiolan-3-one, 2-methyl
	Thiophen-3(2H)-one, dihydro-2-methyl
	dihydro-2-methylthiophen-3(2H)-one
Inchi:	InChI=1S/C5H8OS/c1-4-5(6)2-3-7-4/h4H,2-3H2,1H3
InchiKey:	YMZZPMVKABUEBL-UHFFFAOYSA-N
Formula:	C5H8OS
SMILES:	CC1SCCC1=O
Mol. weight [g/mol]:	116.18

Physical Properties

Property code	Value	Unit	Source
hfus	5.81	kJ/mol	Joback Method
ie	8.75	eV	Cheméo Relay (1.0)
logp	1.081		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
rinpol	1017.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	1000.00		NIST Webbook

rinpol	1011.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	989.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	949.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	999.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	990.00	NIST Webbook
ripol	1512.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1523.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1518.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1561.00	NIST Webbook
ripol	1551.00	NIST Webbook
ripol	1557.00	NIST Webbook
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ripol	1548.00	NIST Webbook

ripol	1565.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1518.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1509.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1528.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1535.00	NIST Webbook
ripol	1538.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.02	J/mol×K	444.73	Joback Method
cpg	180.14	J/mol×K	484.28	Joback Method
cpg	191.71	J/mol×K	523.84	Joback Method
cpg	202.73	J/mol×K	563.39	Joback Method
cpg	213.20	J/mol×K	602.94	Joback Method
cpg	223.10	J/mol×K	642.49	Joback Method
cpg	232.43	J/mol×K	682.05	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679851&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices