

3-methyl-2-oxo-2,5-dihydro-thiophene

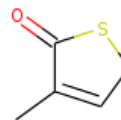
InChI: InChI=1S/C5H6OS/c1-4-2-3-7-5(4)6/h2H,3H2,1H3

InChI Key: XZLYVPCODCYIHS-UHFFFAOYSA-N

Formula: C5H6OS

SMILES: CC1=CCSC1=O

Molecular Weight: 114.17



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-26.92	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-111.84	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	5.57	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	38.30	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.21		Crippen Method
P_c	4856.20	kPa	Joback Method
T_{boil}	453.54	K	Joback Method
T_c	695.30	K	Joback Method
T_{fus}	326.20	K	Joback Method
V_c	0.30	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	152.25	J/mol×K	453.54	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C5H6OS/c1-4-2-3-7-5\(4\)6/h2H,3H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C5H6OS/c1-4-2-3-7-5(4)6/h2H,3H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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