

trans-1-Methoxy-1-butene

Other names: (1E)-1-Butenyl methyl ether; (E)-1-Methoxy-1-butene; (E)-CH₃CH₂CH=CH(OCH₃).

InChI: InChI=1S/C5H10O/c1-3-4-5-6-2/h4-5H,3H2,1-2H3/b5-4+

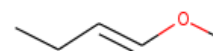
InChI Key: KMQWOHBHEYVPGQJ-SNAWJCMRSA-N

Formula: C₅H₁₀O

SMILES: CCC=COC

Molecular Weight: 86.13

CAS: 10034-13-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-33.56	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-161.53	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	10.10	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	29.09	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.56		Crippen Method
P_c	3615.89	kPa	Joback Method
T_{boil}	340.38	K	Joback Method
T_c	513.77	K	Joback Method
T_{fus}	163.26	K	Joback Method
V_c	0.31	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	133.95	J/mol×K	340.38	Joback Method
η	0.00	Paxs	340.38	Joback Method

Sources

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

NIST Webbook:

<http://webbook.nist.gov/cgi/inchi/InChI=1S/C5H10O/c1-3-4-5-6-2/h4-5H,3H2,1-2H3/b5-4+>

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

Legend

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

η : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$: 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).

$logP_{oct/wat}$: 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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