

1-Butene, 3-methyl-1-(1-propenyloxy)-, (Z,Z)-

InChI: InChI=1S/C8H14O/c1-4-6-9-7-5-8(2)3/h4-8H,1-3H3/b6-4-,7-5-

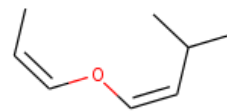
InChI Key: NTDALFWHPAORIU-PEPZGXQESA-N

Formula: C8H14O

SMILES: CC=COC=CC(C)C

Molecular Weight: 126.20

CAS: 61463-35-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	69.48	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-111.51	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	14.54	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	35.34	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.71		Crippen Method
P_c	2796.51	kPa	Joback Method
T_{boil}	412.74	K	Joback Method
T_c	597.74	K	Joback Method
T_{fus}	176.99	K	Joback Method
V_c	0.46	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	227.62	J/mol×K	412.74	Joback Method
η	0.00	Paxs	412.74	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H14O/c1-4-6-9-7-5-8\(2\)3/h4-8H,1-3H3/b6-4-,7-5-](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H14O/c1-4-6-9-7-5-8(2)3/h4-8H,1-3H3/b6-4-,7-5-)

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

Legend

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

η : Dynamic viscosity (Pa \times 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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