

But-1-ene-3-yne, 1-ethoxy-

InChI: InChI=1S/C6H8O/c1-3-5-6-7-4-2/h1,5-6H,4H2,2H3/b6-5+

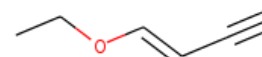
InChI Key: LYWWXPVUSWJFCZ-AATRIKPKSA-N

Formula: C6H8O

SMILES: C#CC=COCC

Molecular Weight: 96.13

CAS: 2806-41-9



Physical Properties

| Property | Value | Unit | Source |
|---------------------------------|---------|------------------------|----------------|
| $\Delta_f G^\circ$ | 197.93 | kJ/mol | Joback Method |
| $\Delta_f H^\circ_{\text{gas}}$ | 109.73 | kJ/mol | Joback Method |
| $\Delta_{\text{fus}} H^\circ$ | 15.66 | kJ/mol | Joback Method |
| $\Delta_{\text{vap}} H^\circ$ | 31.18 | kJ/mol | Joback Method |
| $\log P_{\text{oct/wat}}$ | 1.17 | | Crippen Method |
| P_c | 3853.09 | kPa | Joback Method |
| T_{boil} | 353.38 | K | Joback Method |
| T_c | 539.48 | K | Joback Method |
| T_{fus} | 221.50 | K | Joback Method |
| V_c | 0.33 | m ³ /kg-mol | Joback Method |

Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|--------------------|--------|---------|-----------------|---------------|
| $C_{p,\text{gas}}$ | 146.12 | J/mol×K | 353.38 | Joback Method |

Sources

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

NIST Webbook:

<http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H8O/c1-3-5-6-7-4-2/h1,5-6H,4H2,2H3/b6-5+>

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).

$logP_{oct/wat}$: 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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