

CH₃O[CH₂CH₂CH₂O]₃CH₃

InChI: InChI=1S/C11H24O4/c1-12-6-3-8-14-10-5-11-15-9-4-7-13-2/h3-11
H2,1-2H3

InChI Key: TTYHFEHZJTW HNB-UHFFFAOYSA-N

Formula: C₁₁H₂₄O₄

SMILES: COCCCOCCCOCCCO

Molecular Weight: 220.31

CAS: 66226-75-3



Physical Properties

Property	Value	Unit	Source
BasG	895.10	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	-378.26	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-799.25	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	29.00	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.72	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.48		Crippen Method
P_c	1823.17	kPa	Joback Method
T_{boil}	540.76	K	Joback Method
T_c	702.54	K	Joback Method
T_{fus}	302.65	K	Joback Method
V_c	0.72	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	471.43	J/molxK	540.76	Joback Method
η	0.00	Paxs	540.76	Joback Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H24O4/c1-12-6-3-8-14-10-5-11-15-9-4-7-13-2/h3-11H2,1-2H3>

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

Legend

BasG: Gas basicity (kJ/mol).

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

η: Dynamic viscosity (Pa×s).

Δ_fG°: Standard Gibbs free energy of formation (kJ/mol).

Δ_fH°_{gas}: Enthalpy of formation at standard conditions (kJ/mol).

Δ_{fus}H°: Enthalpy of fusion at standard conditions (kJ/mol).

Δ_{vap}H°: 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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