

Isopropyl-(2-methoxy-ethyl)-propyl-amine

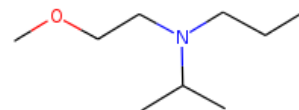
InChI: InChI=1S/C9H21NO/c1-5-6-10(9(2)3)7-8-11-4/h9H,5-8H2,1-4H3

InChI Key: ZZCCSJGBKSBOII-UHFFFAOYSA-N

Formula: C₉H₂₁NO

SMILES: CCCN(CCOC)C(C)C

Molecular Weight: 159.27



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	28.24	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-299.06	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	19.75	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	39.69	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.75		Crippen Method
P_c	2282.77	kPa	Joback Method
T_{boil}	439.74	K	Joback Method
T_c	605.23	K	Joback Method
T_{fus}	230.89	K	Joback Method
V_c	0.57	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	330.44	J/mol×K	439.74	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H21NO/c1-5-6-10\(9\(2\)3\)7-8-11-4/h9H,5-8H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H21NO/c1-5-6-10(9(2)3)7-8-11-4/h9H,5-8H2,1-4H3)

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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