

lys-val

InChI: InChI=1S/C11H23N3O3/c1-7(2)9(11(16)17)14-10(15)8(13)5-3-4-6-12/h7-9H,3-6,12-13H2,1-2H3,(H,14,15)(H,16,17)

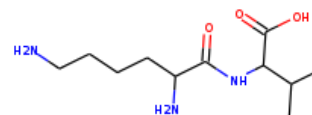
InChI Key: YQAIUOWPSUOINN-UHFFFAOYSA-N

Formula: C11H23N3O3

SMILES: CC(C)C(NC(=O)C(N)CCCCN)C(=O)O

Molecular Weight: 245.32

CAS: 20556-11-0



Physical Properties

Property	Value	Unit	Source
BasG	924.30	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	-137.95	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-542.55	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.46	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	96.80	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	-0.332		Crippen Method
P_c	2755.56	kPa	Joback Method
T_{boil}	844.91	K	Joback Method
T_c	1047.57	K	Joback Method
T_{fus}	548.59	K	Joback Method
V_c	0.757	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	648.34	J/molxK	844.91	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H23N3O3/c1-7\(2\)9\(11\(16\)17\)14-10\(15\)8\(13\)5-3-4-6-12/h7-9H,3-6,12-13H2,1-2H3,\(H,14,15\)\(H,16,17\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H23N3O3/c1-7(2)9(11(16)17)14-10(15)8(13)5-3-4-6-12/h7-9H,3-6,12-13H2,1-2H3,(H,14,15)(H,16,17))

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).

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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