

L-valine, n-heptafluorobutyryl-, pentyl ester

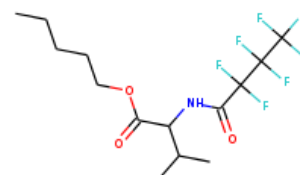
InChI: InChI=1S/C14H20F7NO3/c1-4-5-6-7-25-10(23)9(8(2)3)22-11(24)12(15,16)13(17,18)14(19,20)21/h8-9H,4-7H2,1-3H3,(H,22,24)

InChI Key: RVLMKKYQGZADTK-UHFFFAOYSA-N

Formula: C₁₄H₂₀F₇NO₃

SMILES: CCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C

Molecular Weight: 383.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-1566.48	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-2045.78	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.77	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	58.71	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.69		Crippen Method
P_c	1390.22	kPa	Joback Method
T_{boil}	684.37	K	Joback Method
T_c	850.86	K	Joback Method
T_{fus}	403.68	K	Joback Method
V_c	0.97	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	715.56	J/mol×K	684.37	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H20F7NO3/c1-4-5-6-7-25-10\(23\)9\(8\(2\)3\)22-11\(24\)12\(15,16\)13\(17,18\)14\(19,20\)21/h8-9H,4-7H2,1-3H3,\(H,22,24\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H20F7NO3/c1-4-5-6-7-25-10(23)9(8(2)3)22-11(24)12(15,16)13(17,18)14(19,20)21/h8-9H,4-7H2,1-3H3,(H,22,24))

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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