

L-valine, n-heptafluorobutyryl-, nonyl ester

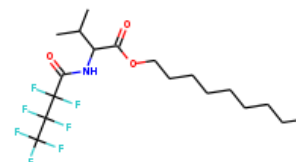
InChI: InChI=1S/C18H28F7NO3/c1-4-5-6-7-8-9-10-11-29-14(27)13(12(2)3)26-15(28)16(19,20)17(21,22)18(23,24)25/h12-13H,4-11H2,1-3H3,(H,26,28)

InChI Key: MZBIKFHJDOTOOB-UHFFFAOYSA-N

Formula: C18H28F7NO3

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

Molecular Weight: 439.41



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-1532.80	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-2128.34	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	44.13	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	67.62	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.25		Crippen Method
P_c	1063.79	kPa	Joback Method
T_{boil}	775.89	K	Joback Method
T_c	951.43	K	Joback Method
T_{fus}	448.76	K	Joback Method
V_c	1.19	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	939.82	J/mol×K	775.89	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H28F7NO3/c1-4-5-6-7-8-9-10-11-29-14\(27\)13\(12\(2\)3\)26-15\(28\)16\(19,20\)17\(21,22\)18\(23,24\)25/h12-13H,4-11H2,1-3H3,\(H,26,28\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H28F7NO3/c1-4-5-6-7-8-9-10-11-29-14(27)13(12(2)3)26-15(28)16(19,20)17(21,22)18(23,24)25/h12-13H,4-11H2,1-3H3,(H,26,28))

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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