

1-tert-Butoxy-2-propanol, heptafluorobutyrate

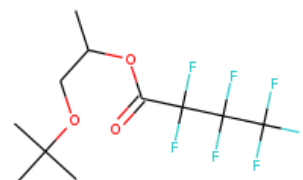
InChI: InChI=1S/C11H15F7O3/c1-6(5-20-8(2,3)4)21-7(19)9(12,13)10(14,15)11(16,17)18/h6H,5H2,1-4H3

InChI Key: TTXDLKZACJODPX-UHFFFAOYSA-N

Formula: C11H15F7O3

SMILES: CC(COC(C)(C)C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Molecular Weight: 328.22



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-1651.93	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-2060.44	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	16.60	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	40.36	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.566		Crippen Method
P_c	1631.17	kPa	Joback Method
T_{boil}	531.32	K	Joback Method
T_c	689.39	K	Joback Method
T_{fus}	306.93	K	Joback Method
V_c	0.769	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	511.48	J/mol×K	531.32	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H15F7O3/c1-6\(5-20-8\(2,3\)4\)21-7\(19\)9\(12,13\)10\(14,15\)11\(16,17\)18/h6H,5H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H15F7O3/c1-6(5-20-8(2,3)4)21-7(19)9(12,13)10(14,15)11(16,17)18/h6H,5H2,1-4H3)

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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