

# 1-tert-Butoxy-2-propanol, heptafluorobutyrate

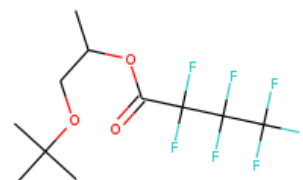
**InChI:** InChI=1S/C11H15F7O3/c1-6(5-20-8(2,3)4)21-7(19)9(12,13)10(14,15)11(16,17)18/h6H,5H2,1-4H3

**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
$T_{\text{boil}}$	531.32	K	Joback Method
$T_c$	689.39	K	Joback Method
$T_{\text{fus}}$	306.93	K	Joback Method
$V_c$	0.769	m <sup>3</sup> /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](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 (m<sup>3</sup>/kg-mol).

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