

Propyl 2-fluorobenzoate

Other names: 2-Fluorobenzoic acid, propyl ester; Benzoic acid, 2-fluoro-, propyl ester.

InChI: InChI=1S/C10H11FO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3

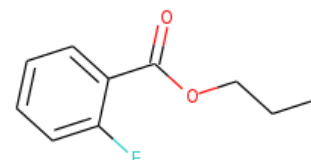
InChI Key: IOQAFIPZQVBMK-UHFFFAOYSA-N

Formula: C10H11FO2

SMILES: CCCOC(=O)c1ccccc1F

Molecular Weight: 182.19

CAS: 811465-80-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-292.63	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-465.58	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	21.18	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	49.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.39		Crippen Method
P_c	2887.40	kPa	Joback Method
T_{boil}	535.42	K	Joback Method
T_c	738.70	K	Joback Method
T_{fus}	314.15	K	Joback Method
V_c	0.53	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	308.55	J/mol×K	535.42	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H11FO2/c1-2-7-13-10\(12\)8-5-3-4-6-9\(8\)11/h3-6H,2,7H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H11FO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3)

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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