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: IOQAFIPZQVBMTK-UHFFFAOYSA-N

Formula: C10H11FO2

SMILES: CCCOC(=O)c1ccccc1F

Molecular Weight: 182.19

CAS: 811465-80-2

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-292.63	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-465.58	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.18	kJ/mol	Joback Method
$\Delta_{vap} H°$	49.13	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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^3/kg-mol).