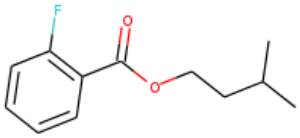
2-Fluorobenzoic acid, 3-methylbutyl ester

InChI: InChI=1S/C12H15FO2/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-6,9H,7-8H2,1-2H3
InChI Key: CQOFKUHFJAYIOP-UHFFFAOYSA-N
Formula: C12H15FO2
SMILES: CC(C)CCOC(=O)c1ccccc1F
Molecular Weight: 210.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-278.23	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-512.14	kJ/mol	Joback Method
$\Delta_{fus} H°$	22.83	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.19	kJ/mol	Joback Method
$logP_{oct/wat}$	3.03		Crippen Method
P_c	2391.19	kPa	Joback Method
T_{boil}	580.74	K	Joback Method
T_c	782.26	K	Joback Method
T_{fus}	321.69	K	Joback Method
V_c	0.64	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	402.33	J/mol×K	580.74	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15FO2/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-6,9H,7-8H2,1-2H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).