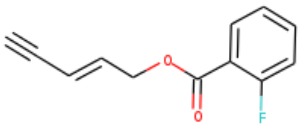
2-Fluorobenzoic acid, pent-2-en-4-ynyl ester

InChI: InChI=1S/C12H9FO2/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h1,3-8H,9H2
InChI Key: WXLWTLPDTMCDCC-UHFFFAOYSA-N
Formula: C12H9FO2
SMILES: C#CC=CCOC(=O)c1ccccc1F
Molecular Weight: 204.20



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	27.50	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-97.74	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.53	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.40	kJ/mol	Joback Method
$logP_{oct/wat}$	2.17		Crippen Method
P_c	2912.39	kPa	Joback Method
T_{boil}	575.46	K	Joback Method
T_c	795.61	K	Joback Method
T_{fus}	378.58	K	Joback Method
V_c	0.58	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	342.59	J/mol×K	575.46	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H9FO2/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h1,3-8H,9H2

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).

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