2,6-Difluoro-3-methylbenzoic acid, 2-ethoxyethyl ester

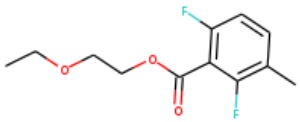
InChI: InChI=1S/C12H14F2O3/c1-3-16-6-7-17-12(15)10-9(13)5-4-8(2)11(10)14/h4-5H,3,6-7H2,1-2H3

InChI Key: JKLGZVWNLXTWJO-UHFFFAOYSA-N

Formula: C12H14F2O3

SMILES: CCOCCOC(=O)c1c(F)ccc(C)c1F

Molecular Weight: 244.23



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-594.86	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-858.13	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.85	kJ/mol	Joback Method
$\Delta_{vap} H°$	56.50	kJ/mol	Joback Method
$logP_{oct/wat}$	2.47		Crippen Method
P_c	2173.43	kPa	Joback Method
T_{boil}	612.83	K	Joback Method
T_c	802.33	K	Joback Method
T_{fus}	384.55	K	Joback Method
V_c	0.68	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	434.50	J/mol×K	612.83	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H14F2O3/c1-3-16-6-7-17-12(15)10-9(13)5-4-8(2)11(10)14/h4-5H,3,6-7H2,1-2H3

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).