

Succinic acid, 1-(2-fluorophenyl)ethyl heptyl ester

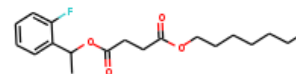
InChI: InChI=1S/C19H27FO4/c1-3-4-5-6-9-14-23-18(21)12-13-19(22)24-15(2)16-10-7-8-11-17(16)20/h7-8,10-11,15H,3-6,9,12-14H2,1-2H3

InChI Key: SDXBCSZHGZUTRK-UHFFFAOYSA-N

Formula: C19H27FO4

SMILES: CCCCCCOC(=O)CCC(=O)OC(C)c1ccccc1F

Molecular Weight: 338.41



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-453.21	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-901.42	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	43.75	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	77.93	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.72		Crippen Method
P_c	1401.69	kPa	Joback Method
T_{boil}	817.19	K	Joback Method
T_c	1014.05	K	Joback Method
T_{fus}	472.74	K	Joback Method
V_c	1.05	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	827.05	J/mol×K	817.19	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H27FO4/c1-3-4-5-6-9-14-23-18\(21\)12-13-19\(22\)24-15\(2\)16-10-7-8-11-17\(16\)20/h7-8,10-11,15H,3-6,9,12-14H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H27FO4/c1-3-4-5-6-9-14-23-18(21)12-13-19(22)24-15(2)16-10-7-8-11-17(16)20/h7-8,10-11,15H,3-6,9,12-14H2,1-2H3)

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).

$logP_{oct/wat}$: 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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