

# Glutaric acid, di(1-(2,6-difluorophenyl)ethyl) ester

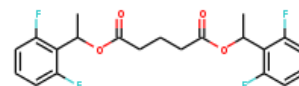
**InChI:** InChI=1S/C21H20F4O4/c1-12(20-14(22)6-3-7-15(20)23)28-18(26)10-5-11-19(27)29-13(2)21-16(24)8-4-9-17(21)25/h3-4,6-9,12-13H,5,10-11H2,1-2H3

**InChI Key:** CHIFOAZRJHRVLT-UHFFFAOYSA-N

**Formula:** C<sub>21</sub>H<sub>20</sub>F<sub>4</sub>O<sub>4</sub>

**SMILES:** CC(OC(=O)CCCC(=O)OC(C)c1c(F)cccc1F)c1c(F)cccc1F

**Molecular Weight:** 412.37



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-939.72	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1334.19	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	47.52	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	83.81	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.32		Crippen Method
$P_c$	1367.69	kPa	Joback Method
$T_{\text{boil}}$	901.94	K	Joback Method
$T_c$	1112.05	K	Joback Method
$T_{\text{fus}}$	546.03	K	Joback Method
$V_c$	1.10	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	865.81	J/mol×K	901.94	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H20F4O4/c1-12\(20-14\(22\)6-3-7-15\(20\)23\)28-18\(26\)10-5-11-19\(27\)29-13\(2\)21-16\(24\)8-4-9-17\(21\)25/h3-4,6-9,12-13H,5,10-11H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H20F4O4/c1-12(20-14(22)6-3-7-15(20)23)28-18(26)10-5-11-19(27)29-13(2)21-16(24)8-4-9-17(21)25/h3-4,6-9,12-13H,5,10-11H2,1-2H3)

**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 (m<sup>3</sup>/kg-mol).

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