

# Succinic acid, 4-fluorobenzyl isobutyl ester

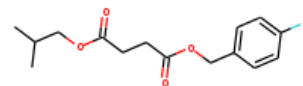
**InChI:** InChI=1S/C15H19FO4/c1-11(2)9-19-14(17)7-8-15(18)20-10-12-3-5-13(16)6-4-12/h3-6,11H,7-10H2,1-2H3

**InChI Key:** IYTHZLPQHIZCKO-UHFFFAOYSA-N

**Formula:** C15H19FO4

**SMILES:** CC(C)COC(=O)CCC(=O)OCc1ccc(F)cc1

**Molecular Weight:** 282.31



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-486.89	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-818.86	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.39	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	69.03	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.85		Crippen Method
$P_c$	1911.91	kPa	Joback Method
$T_{\text{boil}}$	725.67	K	Joback Method
$T_c$	925.21	K	Joback Method
$T_{\text{fus}}$	427.66	K	Joback Method
$V_c$	0.83	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	601.99	J/mol×K	725.67	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/C15H19FO4/c1-11\(2\)9-19-14\(17\)7-8-15\(18\)20-10-12-3-5-13\(16\)6-4-12/h3-6,11H,7-10H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19FO4/c1-11(2)9-19-14(17)7-8-15(18)20-10-12-3-5-13(16)6-4-12/h3-6,11H,7-10H2,1-2H3)

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

## 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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