

Glutaric acid, 2-fluorobenzyl isobutyl ester

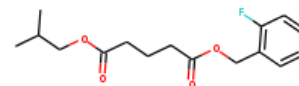
InChI: InChI=1S/C16H21FO4/c1-12(2)10-20-15(18)8-5-9-16(19)21-11-13-6-3-4-7-14(13)17/h3-4,6-7,12H,5,8-11H2,1-2H3

InChI Key: GXBKJFFNTMVWCL-UHFFFAOYSA-N

Formula: C16H21FO4

SMILES: CC(C)COC(=O)CCCC(=O)OCc1ccccc1F

Molecular Weight: 296.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-478.47	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-839.50	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.98	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.25	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.24		Crippen Method
P_c	1760.97	kPa	Joback Method
T_{boil}	748.55	K	Joback Method
T_c	946.59	K	Joback Method
T_{fus}	438.93	K	Joback Method
V_c	0.88	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	656.73	J/mol×K	748.55	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21FO4/c1-12\(2\)10-20-15\(18\)8-5-9-16\(19\)21-11-13-6-3-4-7-14\(13\)17/h3-4,6-7,12H,5,8-11H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21FO4/c1-12(2)10-20-15(18)8-5-9-16(19)21-11-13-6-3-4-7-14(13)17/h3-4,6-7,12H,5,8-11H2,1-2H3)

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).

$\log P_{oct/wat}$: 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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