

Glutaric acid, 2-fluorobenzyl pentyl ester

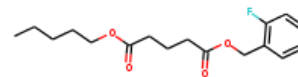
InChI: InChI=1S/C17H23FO4/c1-2-3-6-12-21-16(19)10-7-11-17(20)22-13-14-8-4-5-9-15(14)18/h4-5,8-9H,2-3,6-7,10-13H2,1H3

InChI Key: WCXNNZNBNYTGBW-UHFFFAOYSA-N

Formula: C17H23FO4

SMILES: CCCCCOC(=O)CCCC(=O)OCc1ccccc1F

Molecular Weight: 310.36



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-467.61	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-854.86	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	42.09	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	73.87	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.77		Crippen Method
P_c	1616.77	kPa	Joback Method
T_{boil}	771.87	K	Joback Method
T_c	966.58	K	Joback Method
T_{fus}	465.20	K	Joback Method
V_c	0.95	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	711.99	J/mol×K	771.87	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H23FO4/c1-2-3-6-12-21-16\(19\)10-7-11-17\(20\)22-13-14-8-4-5-9-15\(14\)18/h4-5,8-9H,2-3,6-7,10-13H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H23FO4/c1-2-3-6-12-21-16(19)10-7-11-17(20)22-13-14-8-4-5-9-15(14)18/h4-5,8-9H,2-3,6-7,10-13H2,1H3)

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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