

Glutaric acid, butyl 2-fluorobenzyl ester

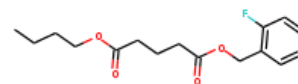
InChI: InChI=1S/C16H21FO4/c1-2-3-11-20-15(18)9-6-10-16(19)21-12-13-7-4-5-8-14(13)17/h4-5,7-8H,2-3,6,9-12H2,1H3

InChI Key: UQKBHVDPIGPDDA-UHFFFAOYSA-N

Formula: C16H21FO4

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

Molecular Weight: 296.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-476.03	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-834.22	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.50	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.38		Crippen Method
P_c	1749.21	kPa	Joback Method
T_{boil}	748.99	K	Joback Method
T_c	944.39	K	Joback Method
T_{fus}	453.93	K	Joback Method
V_c	0.89	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	656.18	J/mol×K	748.99	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21FO4/c1-2-3-11-20-15\(18\)9-6-10-16\(19\)21-12-13-7-4-5-8-14\(13\)17/h4-5,7-8H,2-3,6,9-12H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21FO4/c1-2-3-11-20-15(18)9-6-10-16(19)21-12-13-7-4-5-8-14(13)17/h4-5,7-8H,2-3,6,9-12H2,1H3)

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).

$\log P_{oct/wat}$: 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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