Glutaric acid, butyl 4-fluorobenzyl ester

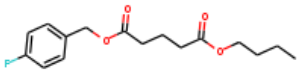
InChI: InChI=1S/C16H21FO4/c1-2-3-11-20-15(18)5-4-6-16(19)21-12-13-7-9-14(17)10-8-13/h7-10H,2-6,11-12H2,1H3

InChI Key: RLRGJPOGNUPZFR-UHFFFAOYSA-N

Formula: C16H21FO4

SMILES: CCCCOC(=O)CCCC(=O)OCc1ccc(F)cc1

Molecular Weight: 296.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-476.03	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-834.22	kJ/mol	Joback Method
$\Delta_{fus} H°$	39.50	kJ/mol	Joback Method
$\Delta_{vap} H°$	71.64	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	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)5-4-6-16(19)21-12-13-7-9-14(17)10-8-13/h7-10H,2-6,11-12H2,1H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).