Glutaric acid, butyl 2,5-difluorobenzyl ester

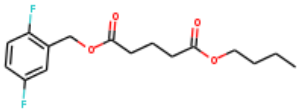
InChI: InChI=1S/C16H20F2O4/c1-2-3-9-21-15(19)5-4-6-16(20)22-11-12-10-13(17)7-8-14(12)18/h7-8,10H,2-6,9,11H2,1H3

InChI Key: VJOZFPPDQXOBLU-UHFFFAOYSA-N

Formula: C16H20F2O4

SMILES: CCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1F

Molecular Weight: 314.32



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-680.47	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1041.80	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.19	kJ/mol	Joback Method
$\Delta_{vap} H°$	71.49	kJ/mol	Joback Method
$logP_{oct/wat}$	3.52		Crippen Method
P_c	1664.61	kPa	Joback Method
T_{boil}	753.24	K	Joback Method
T_c	943.80	K	Joback Method
T_{fus}	467.04	K	Joback Method
V_c	0.91	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	663.08	J/mol×K	753.24	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H20F2O4/c1-2-3-9-21-15(19)5-4-6-16(20)22-11-12-10-13(17)7-8-14(12)18/h7-8,10H,2-6,9,11H2,1H3

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).