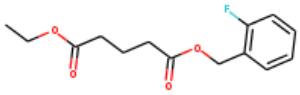
Glutaric acid, ethyl 2-fluorobenzyl ester

InChI: InChI=1S/C14H17FO4/c1-2-18-13(16)8-5-9-14(17)19-10-11-6-3-4-7-12(11)15/h3-4,6-7H,2,5,8-10H2,1H3
InChI Key: XDRWBEGHPGNWTL-UHFFFAOYSA-N
Formula: C14H17FO4
SMILES: CCOC(=O)CCCC(=O)OCc1ccccc1F
Molecular Weight: 268.28



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-492.87	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-792.94	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.32	kJ/mol	Joback Method
$\Delta_{vap} H°$	67.19	kJ/mol	Joback Method
$logP_{oct/wat}$	2.60		Crippen Method
P_c	2068.00	kPa	Joback Method
T_{boil}	703.23	K	Joback Method
T_c	901.55	K	Joback Method
T_{fus}	431.39	K	Joback Method
V_c	0.78	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	547.87	J/mol×K	703.23	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H17FO4/c1-2-18-13(16)8-5-9-14(17)19-10-11-6-3-4-7-12(11)15/h3-4,6-7H,2,5,8-10H2,1H3

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).