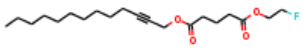
Glutaric acid, tridec-2-yn-1-yl 2-fluoroethyl ester

InChI: InChI=1S/C20H33FO4/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-19(22)14-13-15-20(23)25-18-16-21/h2-10,13-18H2,1H3
InChI Key: QFCHFMRADNWQGM-UHFFFAOYSA-N
Formula: C20H33FO4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCF
Molecular Weight: 356.47



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-342.33	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-869.54	kJ/mol	Joback Method
$\Delta_{fus} H°$	59.33	kJ/mol	Joback Method
$\Delta_{vap} H°$	79.76	kJ/mol	Joback Method
$logP_{oct/wat}$	4.75		Crippen Method
P_c	1164.04	kPa	Joback Method
T_{boil}	817.85	K	Joback Method
T_c	1005.74	K	Joback Method
T_{fus}	566.17	K	Joback Method
V_c	1.18	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	927.21	J/mol×K	817.85	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H33FO4/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-19(22)14-13-15-20(23)25-18-16-21/h2-10,13-18H2,1H3

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).