Diethylmalonic acid, decyl 2,4,5-trifluorobenzyl ester

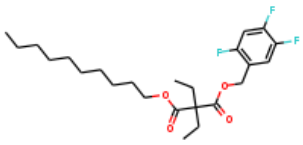
InChI: InChI=1S/C24H35F3O4/c1-4-7-8-9-10-11-12-13-14-30-22(28)24(5-2,6-3)23(29)31-17-18-15-20(26)21(27)16-19(18)25/h15-16H,4-14,17H2,1-3H3

InChI Key: CWVJZXQWABWAQC-UHFFFAOYSA-N

Formula: C24H35F3O4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)cc1F

Molecular Weight: 444.53



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-814.71	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1423.25	kJ/mol	Joback Method
$\Delta_{fus} H°$	58.19	kJ/mol	Joback Method
$\Delta_{vap} H°$	87.85	kJ/mol	Joback Method
$logP_{oct/wat}$	6.64		Crippen Method
P_c	940.95	kPa	Joback Method
T_{boil}	937.30	K	Joback Method
T_c	1147.65	K	Joback Method
T_{fus}	572.73	K	Joback Method
V_c	1.36	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1139.37	J/mol×K	937.3	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H35F3O4/c1-4-7-8-9-10-11-12-13-14-30-22(28)24(5-2,6-3)23(29)31-17-18-15-20(26)21(27)16-19(18)25/h15-16H,4-14,17H2,1-3H3

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).