

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

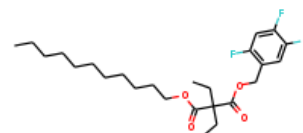
InChI: InChI=1S/C25H37F3O4/c1-4-7-8-9-10-11-12-13-14-15-31-23(29)25(5-2,6-3)24(30)32-18-19-16-21(27)22(28)17-20(19)26/h16-17H,4-15,18H,2,1-3H3

InChI Key: BQBDRCXRXZDMOJ-UHFFFAOYSA-N

Formula: C₂₅H₃₇F₃O₄

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

Molecular Weight: 458.55



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-806.29	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1443.89	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	60.78	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	90.07	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	7.03		Crippen Method
P_c	887.88	kPa	Joback Method
T_{boil}	960.18	K	Joback Method
T_c	1176.72	K	Joback Method
T_{fus}	584.00	K	Joback Method
V_c	1.42	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1200.84	J/mol×K	960.18	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H37F3O4/c1-4-7-8-9-10-11-12-13-14-15-31-23\(29\)25\(5-2,6-3\)24\(30\)32-18-19-16-21\(27\)22\(28\)17-20\(19\)26/h16-17H,4-15,18H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H37F3O4/c1-4-7-8-9-10-11-12-13-14-15-31-23(29)25(5-2,6-3)24(30)32-18-19-16-21(27)22(28)17-20(19)26/h16-17H,4-15,18H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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