Diethylmalonic acid, di(4-trifluoromethylbenzyl) ester

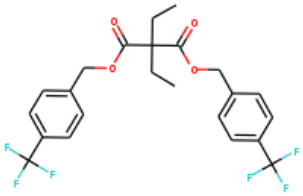
InChI: InChI=1S/C23H22F6O4/c1-3-21(4-2,19(30)32-13-15-5-9-17(10-6-15)22(24,25)26)20(31)33-14-16-7-11-18(12-8-16)23(27,28)29/h5-12H,3-4,13-14H2,1-2H3

InChI Key: MCWGFITXDWIRIW-UHFFFAOYSA-N

Formula: C23H22F6O4

SMILES: CCC(CC)(C(=O)OCc1ccc(C(F)(F)F)cc1)C(=O)OCc1ccc(C(F)(F)F)cc1

Molecular Weight: 476.41



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1279.84	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1760.44	kJ/mol	Joback Method
$\Delta_{fus} H°$	44.44	kJ/mol	Joback Method
$\Delta_{vap} H°$	82.19	kJ/mol	Joback Method
$logP_{oct/wat}$	6.32		Crippen Method
P_c	1176.85	kPa	Joback Method
T_{boil}	927.47	K	Joback Method
T_c	1140.44	K	Joback Method
T_{fus}	581.97	K	Joback Method
V_c	1.23	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	999.90	J/mol×K	927.47	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H22F6O4/c1-3-21(4-2,19(30)32-13-15-5-9-17(10-6-15)22(24,25)26)20(31)33-14-16-7-11-18(12-8-16)23(27,28)29/h5-12H,3-4,13-14H2,1-2H3

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).