Diethylmalonic acid, 2,2,3,3,4,4,4-heptafluorobutyl heptyl ester

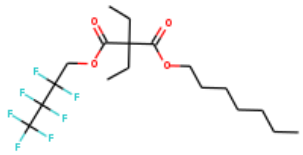
InChI: InChI=1S/C18H27F7O4/c1-4-7-8-9-10-11-28-13(26)15(5-2,6-3)14(27)29-12-16(19,20)17(21,22)18(23,24)25/h4-12H2,1-3H3

InChI Key: BGICUZPKOFZWII-UHFFFAOYSA-N

Formula: C18H27F7O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Molecular Weight: 440.39



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1719.47	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-2312.22	kJ/mol	Joback Method
$\Delta_{fus} H°$	39.85	kJ/mol	Joback Method
$\Delta_{vap} H°$	63.07	kJ/mol	Joback Method
$logP_{oct/wat}$	5.68		Crippen Method
P_c	1045.30	kPa	Joback Method
T_{boil}	745.79	K	Joback Method
T_c	916.58	K	Joback Method
T_{fus}	450.75	K	Joback Method
V_c	1.17	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	909.63	J/mol×K	745.79	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H27F7O4/c1-4-7-8-9-10-11-28-13(26)15(5-2,6-3)14(27)29-12-16(19,20)17(21,22)18(23,24)25/h4-12H2,1-3H3

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).