

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

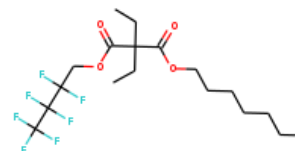
InChI: InChI=1S/C18H27F7O4/c1-4-7-8-9-10-11-28-13(26)15(5-2,6-3)14(27)29-12-16(19,20)17(21,22)18(23,24)25/h4-12H2,1-3H3

InChI Key: BGICUZPKOFZWII-UHFFFAOYSA-N

Formula: C18H27F7O4

SMILES: CCCCCCOC(=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
$\Delta_f G^\circ$	-1719.47	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-2312.22	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.85	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	63.07	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	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](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/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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