Tetrabis(2,2,2-trinitroethyl(orthocarbonate

InChI: InChI=1S/C9H8N12O28/c22-10(23)5(11(24)25,12(26)27)1-46-9(47-2-6(13(28)29,14(30)31)15(32)33,48-3-7(16(34)35,17(36)37)18(38)39)49-4-8(19(40)41,20(42)43)21(44)45/h1-4H2

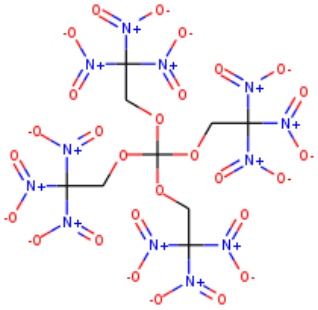
InChI Key: JPTHXHQVODRICI-UHFFFAOYSA-N

Formula: C9H8N12O28

SMILES: O=[N+]([O-])C(COC(OCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])(OCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])OCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]

Molecular Weight: 732.22

CAS: 14548-58-4



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-3918.00 ± 4.20	kJ/mol	NIST Webbook
$\Delta_f G°$	45.70	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-930.84	kJ/mol	Joback Method
$\Delta_f H°_{solid}$	-766.90 ± 4.20	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	123.08	kJ/mol	Joback Method
$\Delta_{sub} H°$	179.00	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	237.88	kJ/mol	Joback Method
$logP_{oct/wat}$	-4.40		Crippen Method
P_c	2738.28	kPa	Joback Method
T_{boil}	2300.93	K	Joback Method
T_c	2991.35	K	Joback Method
T_{fus}	2015.53	K	Joback Method
V_c	1.54	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1752.99	J/mol×K	2300.93	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H8N12O28/c22-10(23)5(11(24)25,12(26)27)1-46-9(47-2-6(13(28)29,14(30)31)15(32)33,48-3-7(16(34)35,17(36)37)18(38)39)49-4-8(19(40)41,20(42)43)21(44)45/h1-4H2

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

Δ_c**H°**$_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{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).