

Adipic acid, ethyl 2,2,2-trichloroethyl ester

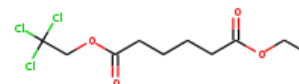
InChI: InChI=1S/C10H15Cl3O4/c1-2-16-8(14)5-3-4-6-9(15)17-7-10(11,12)13/h2-7H2,1H3

InChI Key: NEAFJDMKYTVQND-UHFFFAOYSA-N

Formula: C10H15Cl3O4

SMILES: CCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl

Molecular Weight: 305.58



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-467.47	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-795.30	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.41	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	68.02	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.02		Crippen Method
P_c	2108.07	kPa	Joback Method
T_{boil}	689.84	K	Joback Method
T_c	891.41	K	Joback Method
T_{fus}	438.96	K	Joback Method
V_c	0.78	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	497.68	J/mol×K	689.84	Joback Method
η	0.00	Paxs	689.84	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H15Cl3O4/c1-2-16-8\(14\)5-3-4-6-9\(15\)17-7-10\(11,12\)13/h2-7H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H15Cl3O4/c1-2-16-8(14)5-3-4-6-9(15)17-7-10(11,12)13/h2-7H2,1H3)

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

Legend

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

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: 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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