

Terephthalic acid, di(2,2-dichloroethyl) ester

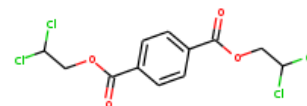
InChI: InChI=1S/C12H10Cl4O4/c13-9(14)5-19-11(17)7-1-2-8(4-3-7)12(18)20-6-10(15)16/h1-4,9-10H,5-6H2

InChI Key: CGYYTTZDBWJDMS-UHFFFAOYSA-N

Formula: C12H10Cl4O4

SMILES: O=C(OCC(Cl)Cl)c1ccc(C(=O)OCC(Cl)Cl)cc1

Molecular Weight: 360.02



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-367.50	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-629.07	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.80	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.32	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.61		Crippen Method
P_c	2280.59	kPa	Joback Method
T_{boil}	807.04	K	Joback Method
T_c	1038.33	K	Joback Method
T_{fus}	497.94	K	Joback Method
V_c	0.83	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	528.04	J/mol×K	807.04	Joback Method
η	0.00	Paxs	807.04	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10Cl4O4/c13-9\(14\)5-19-11\(17\)7-1-2-8\(4-3-7\)12\(18\)20-6-10\(15\)16/h1-4,9-10H,5-6H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10Cl4O4/c13-9(14)5-19-11(17)7-1-2-8(4-3-7)12(18)20-6-10(15)16/h1-4,9-10H,5-6H2)

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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