

Fumaric acid, nonyl 2,2,2-trichloroethyl ester

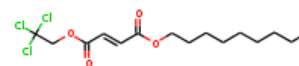
InChI: InChI=1S/C15H23Cl3O4/c1-2-3-4-5-6-7-8-11-21-13(19)9-10-14(20)22-12-15(16,17)18/h9-10H,2-8,11-12H2,1H3/b10-9+

InChI Key: JRFRJYDZGXWGQR-MDZDMXLPSA-N

Formula: C15H23Cl3O4

SMILES: CCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl

Molecular Weight: 373.70



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-345.15	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-781.28	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	45.56	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	79.11	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.75		Crippen Method
P_c	1472.49	kPa	Joback Method
T_{boil}	808.40	K	Joback Method
T_c	1008.92	K	Joback Method
T_{fus}	490.23	K	Joback Method
V_c	1.04	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	739.95	J/mol×K	808.4	Joback Method
η	0.00	Paxs	808.4	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H23Cl3O4/c1-2-3-4-5-6-7-8-11-21-13\(19\)9-10-14\(20\)22-12-15\(16,17\)18/h9-10H,2-8,11-12H2,1H3/b10-9+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H23Cl3O4/c1-2-3-4-5-6-7-8-11-21-13(19)9-10-14(20)22-12-15(16,17)18/h9-10H,2-8,11-12H2,1H3/b10-9+)

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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