

Dibenzodioxin, 1,2,8,9-tetrabromo-, 3,7-dichloro-

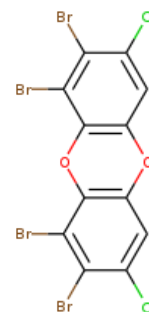
InChI: InChI=1S/C12H2Br4Cl2O2/c13-7-3(17)1-5-11(9(7)15)20-12-6(19-5)2-4(18)8(14)10(12)16/h1-2H

InChI Key: CJEHQTSAYMHKIS-UHFFFAOYSA-N

Formula: C12H2Br4Cl2O2

SMILES: Clc1cc2c(c(Br)c1Br)Oc1c(Br)c(Br)c(Cl)cc1O2

Molecular Weight: 568.66



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	139.68	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-0.57	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	56.46	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	95.73	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	7.94		Crippen Method
P_c	4409.10	kPa	Joback Method
T_{boil}	967.70	K	Joback Method
T_c	1266.25	K	Joback Method
T_{fus}	755.88	K	Joback Method
V_c	0.85	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	435.76	J/mol×K	967.7	Joback Method
η	0.00	Paxs	967.7	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H2Br4Cl2O2/c13-7-3\(17\)1-5-11\(9\(7\)15\)20-12-6\(19-5\)2-4\(18\)8\(14\)10\(12\)16/h1-2H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H2Br4Cl2O2/c13-7-3(17)1-5-11(9(7)15)20-12-6(19-5)2-4(18)8(14)10(12)16/h1-2H)

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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