

1,3,6,8-tetrabromo-dibenzo-dioxin

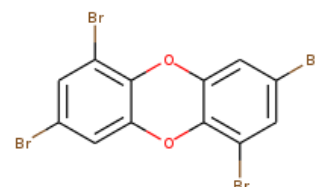
InChI: InChI=1S/C12H4Br4O2/c13-5-1-7(15)11-9(3-5)18-12-8(16)2-6(14)4-10(12)17-11/h1-4H

InChI Key: FLEIILCTHUDZIV-UHFFFAOYSA-N

Formula: C12H4Br4O2

SMILES: BrC1cc(Br)c2c(c1)Oc1c(Br)cc(Br)cc1O2

Molecular Weight: 499.77



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	182.80	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	53.85	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	48.85	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	85.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.63		Crippen Method
P_c	5087.49	kPa	Joback Method
T_{boil}	882.88	K	Joback Method
T_c	1180.48	K	Joback Method
T_{fus}	671.00	K	Joback Method
V_c	0.75	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	412.07	J/mol×K	882.88	Joback Method
η	0.00	Paxs	882.88	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H4Br4O2/c13-5-1-7\(15\)11-9\(3-5\)18-12-8\(16\)2-6\(14\)4-10\(12\)17-11/h1-4H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H4Br4O2/c13-5-1-7(15)11-9(3-5)18-12-8(16)2-6(14)4-10(12)17-11/h1-4H)

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

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol \times K).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: 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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