

Hexane, 1,2,5,6-tetrabromo-

Other names: 1,2,5,6-Tetrabromohexane.

InChI: InChI=1S/C6H10Br4/c7-3-5(9)1-2-6(10)4-8/h5-6H,1-4H2

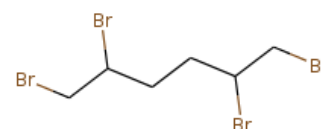
InChI Key: WPBWUVCMCYXPFI-UHFFFAOYSA-N

Formula: C6H10Br4

SMILES: BrCC(Br)CCC(Br)CBr

Molecular Weight: 401.76

CAS: 58443-86-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	52.04	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-72.41	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	25.39	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	53.91	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.08		Crippen Method
P_c	4432.62	kPa	Joback Method
T_{boil}	600.44	K	Joback Method
T_c	841.15	K	Joback Method
T_{fus}	322.65 ± 2.00	K	NIST Webbook
V_c	0.61	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	298.17	J/mol×K	600.44	Joback Method
η	0.00	Paxs	600.44	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H10Br4/c7-3-5\(9\)1-2-6\(10\)4-8/h5-6H,1-4H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H10Br4/c7-3-5(9)1-2-6(10)4-8/h5-6H,1-4H2)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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).

Latest version available from:

<https://www.chemeo.com/cid/62-006-6/Hexane%2C%201%2C2%2C5%2C6-tetrabromo->

Generated by Cheméo on Tue, 29 Sep 2020 11:00:50 +0000.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.