

1,4-Dimethyl-2,3-bis(chloromethyl)benzene

InChI:

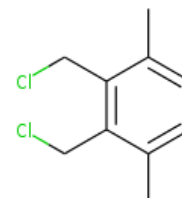
InChI=1S/C10H12Cl2/c1-7-3-4-8(2)10(6-12)9(7)5-11/h3-4H,5-6H2,1-2H3

InChI Key: IVGNPAAPUGCMPW-UHFFFAOYSA-N

Formula: C₁₀H₁₂Cl₂

SMILES: Cc1ccc(C)c(CCl)c1CCl

Molecular Weight: 203.11



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	92.98	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-79.09	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	22.92	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.89	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.78		Crippen Method
P_c	2587.22	kPa	Joback Method
T_{boil}	544.68	K	Joback Method
T_c	763.73	K	Joback Method
T_{fus}	326.28	K	Joback Method
V_c	0.59	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	311.67	J/mol×K	544.68	Joback Method
η	0.00	Paxs	544.68	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12Cl2/c1-7-3-4-8\(2\)10\(6-12\)9\(7\)5-11/h3-4H,5-6H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12Cl2/c1-7-3-4-8(2)10(6-12)9(7)5-11/h3-4H,5-6H2,1-2H3)

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

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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