

Succinic acid, 2,2-dichloroethyl 4-bromophenyl ester

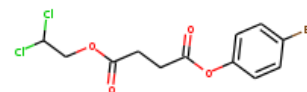
InChI: InChI=1S/C12H11BrCl2O4/c13-8-1-3-9(4-2-8)19-12(17)6-5-11(16)18-7-10(14)15/h1-4,10H,5-7H2

InChI Key: ARBSHKNAUOLACR-UHFFFAOYSA-N

Formula: C12H11BrCl2O4

SMILES: O=C(CCC(=O)Oc1ccc(Br)cc1)OCC(Cl)Cl

Molecular Weight: 370.02



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-326.88	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-565.98	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.22	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.37	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.48		Crippen Method
P_c	2605.74	kPa	Joback Method
T_{boil}	798.78	K	Joback Method
T_c	1030.49	K	Joback Method
T_{fus}	512.90	K	Joback Method
V_c	0.80	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	515.88	J/mol×K	798.78	Joback Method
η	0.00	Paxs	798.78	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11BrCl2O4/c13-8-1-3-9\(4-2-8\)19-12\(17\)6-5-11\(16\)18-7-10\(14\)15/h1-4,10H,5-7H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H11BrCl2O4/c13-8-1-3-9(4-2-8)19-12(17)6-5-11(16)18-7-10(14)15/h1-4,10H,5-7H2)

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

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).

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