

Adipic acid, 2,2-dichloroethyl pentyl ester

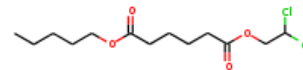
InChI: InChI=1S/C13H22Cl2O4/c1-2-3-6-9-18-12(16)7-4-5-8-13(17)19-10-11(14)15/h11H,2-10H2,1H3

InChI Key: YRKPIUINHGBECT-UHFFFAOYSA-N

Formula: C13H22Cl2O4

SMILES: CCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl

Molecular Weight: 313.22



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-435.56	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-838.01	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.87	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.23	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.63		Crippen Method
P_c	1679.66	kPa	Joback Method
T_{boil}	723.84	K	Joback Method
T_c	911.74	K	Joback Method
T_{fus}	425.43	K	Joback Method
V_c	0.90	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	627.11	J/mol×K	723.84	Joback Method
η	0.00	Paxs	723.84	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H22Cl2O4/c1-2-3-6-9-18-12\(16\)7-4-5-8-13\(17\)19-10-11\(14\)15/h11H,2-10H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H22Cl2O4/c1-2-3-6-9-18-12(16)7-4-5-8-13(17)19-10-11(14)15/h11H,2-10H2,1H3)

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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