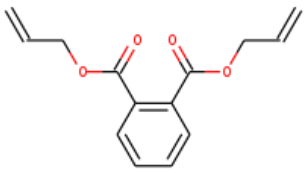
1,2-Benzenedicarboxylic acid, di-2-propenyl ester



Other names: 1,2-Benzenedicarboxylic acid, 1,2-di-2-propen-1-yl ester; 1,2-Benzenedicarboxylic acid, di-2-propenyl ester; Allyl phthalate; DAP monomer; Dapon 35; Dapon R; Diallyl ester o-phthalic acid; Diallyl ester of phthalic acid; Diallylester kyseliny ftalove; Diallylester phthalic acid; NCI-C50657; NSC 7667; Phthalic acid, diallyl ester; o-Phthalic acid, diallyl ester.

InChI: InChI=1S/C14H14O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3-8H,1-2,9-10H2

InChI Key: QUDWYFHPNIMBFC-UHFFFAOYSA-N

Formula: C14H14O4

SMILES: C=CCOC(=O)c1ccccc1C(=O)OCC=C

Molecular Weight: 246.26

CAS: 131-17-9

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-6960.10	kJ/mol	NIST Webbook
$\Delta_c H°_{liquid}$	-6957.60 ± 7.10	kJ/mol	NIST Webbook
$\Delta_f G°$	-122.38	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-345.97	kJ/mol	Joback Method
$\Delta_f H°_{liquid}$	-549.80	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-552.40 ± 7.10	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	28.68	kJ/mol	Joback Method
$\Delta_{vap} H°$	66.67	kJ/mol	Joback Method
$logP_{oct/wat}$	2.37		Crippen Method
P_c	2333.78	kPa	Joback Method
T_{boil}	439.20	K	NIST Webbook
T_c	910.28	K	Joback Method
T_{fus}	427.28	K	Joback Method
V_c	0.72	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	492.72	J/mol×K	697.32	Joback Method
η	0.00	Pa×s	697.32	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H14O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3-8H,1-2,9-10H2

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

Legend

Δ_c**H°**$_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P**$_{oct/wat}$: 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 (m^3/kg-mol).