

2-(Propoxycarbonyl)benzoic acid

Other names: 1,2-Benzenedicarboxylic acid, 1-propyl ester; Monopropyl phthalate; Phthalic acid, monopropyl ester; Propyl hydrogen phthalate.

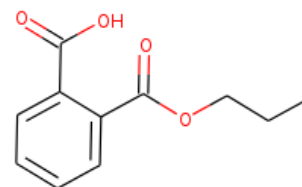
InChI: InChI=1S/C11H12O4/c1-2-7-15-11(14)9-6-4-3-5-8(9)10(12)13/h3-6H,2,7H2,1H3,(H,12,13)

InChI Key: NFOQRXSEYVCJP-UHFFFAOYSA-N

Formula: C11H12O4

SMILES: CCCOC(=O)c1ccccc1C(=O)O

Molecular Weight: 208.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-355.14	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-554.92	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	26.37	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	75.60	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.95		Crippen Method
P_c	3239.34	kPa	Joback Method
T_{boil}	705.08	K	Joback Method
T_c	908.75	K	Joback Method
T_{fus}	435.58	K	Joback Method
V_c	0.59	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	411.52	J/mol×K	705.08	Joback Method
η	0.00	Paxs	705.08	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12O4/c1-2-7-15-11\(14\)9-6-4-3-5-8\(9\)10\(12\)13/h3-6H,2,7H2,1H3,\(H,12,13\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12O4/c1-2-7-15-11(14)9-6-4-3-5-8(9)10(12)13/h3-6H,2,7H2,1H3,(H,12,13))

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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