

Cyclobutanecarboxylic acid, phenyl ester

InChI: InChI=1S/C11H12O2/c12-11(9-5-4-6-9)13-10-7-2-1-3-8-10/h1-3,7-9H,4-6H2

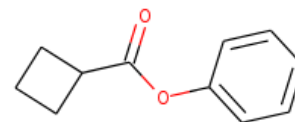
InChI Key: QSPUUVAPVKVXFB-UHFFFAOYSA-N

Formula: C11H12O2

SMILES: O=C(Oc1ccccc1)C1CCC1

Molecular Weight: 176.21

CAS: 30466-31-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-31.12	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-212.00	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	17.11	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.60	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.39		Crippen Method
P_c	3295.37	kPa	Joback Method
T_{boil}	565.06	K	Joback Method
T_c	798.36	K	Joback Method
T_{fus}	326.73	K	Joback Method
V_c	0.52	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	332.53	J/mol×K	565.06	Joback Method
η	0.00	Paxs	565.06	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12O2/c12-11\(9-5-4-6-9\)13-10-7-2-1-3-8-10/h1-3,7-9H,4-6H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12O2/c12-11(9-5-4-6-9)13-10-7-2-1-3-8-10/h1-3,7-9H,4-6H2)

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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