Benzoic acid, 1-naphthyl ester

Other names: 1-Naphthol, benzoate; 1-Naphthyl benzoate; Benzoic acid, 1-naphthyl ester.

InChI: InChI=1S/C17H12O2/c18-17(14-8-2-1-3-9-14)19-16-12-6-10-13-7-4-5-11-15(13)16/h1-12H

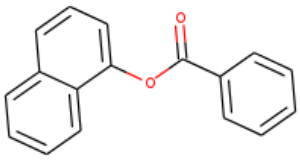
InChI Key: KZWCTFLBFSWYHS-UHFFFAOYSA-N

Formula: C17H12O2

SMILES: O=C(Oc1cccc2ccccc21)c1ccccc1

Molecular Weight: 248.28

CAS: 607-55-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	180.18	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	13.65	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.29	kJ/mol	Joback Method
$\Delta_{vap} H°$	69.45	kJ/mol	Joback Method
IE	7.81	eV	NIST Webbook
$logP_{oct/wat}$	4.06		Crippen Method
P_c	2735.42	kPa	Joback Method
T_{boil}	741.97	K	Joback Method
T_c	998.93	K	Joback Method
T_{fus}	329.00 ± 0.50	K	NIST Webbook
V_c	0.72	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	503.24	J/mol×K	741.97	Joback Method
η	0.00	Pa×s	741.97	Joback Method

Property	Value	Unit	Temperature (K)	Source
$\Delta_{fus}H$	16.98	kJ/mol	329.2	NIST Webbook
$\Delta_{fus}H$	16.98	kJ/mol	329.2	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H12O2/c18-17(14-8-2-1-3-9-14)19-16-12-6-10-13-7-4-5-11-15(13)16/h1-12H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: 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_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***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).