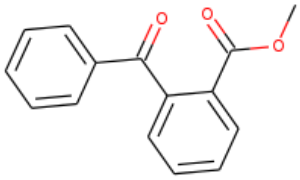
Benzoic acid, 2-benzoyl-, methyl ester

Other names: 2-Benzoylbenzoic acid, methyl ester; Benzoic acid, o-benzoyl-, methyl ester; Methyl o-benzoylbenzoate; Methyl-2-benzoylbenzoate; o-(Methoxycarbonyl)benzophenone; o-Benzoylbenzoic acid methyl ester.



InChI: InChI=1S/C15H12O3/c1-18-15(17)13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10H,1H3

InChI Key: NQSMEZJWJJVYOI-UHFFFAOYSA-N

Formula: C15H12O3

SMILES: COC(=O)c1ccccc1C(=O)c1ccccc1

Molecular Weight: 240.25

CAS: 606-28-0

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-72.23	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-248.72	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.68	kJ/mol	Joback Method
$\Delta_{vap} H°$	70.10	kJ/mol	Joback Method
$log P_{oct/wat}$	2.70		Crippen Method
P_c	2764.26	kPa	Joback Method
T_{boil}	625.00	K	NIST Webbook
T_c	975.09	K	Joback Method
T_{fus}	325.00	K	NIST Webbook
V_c	0.69	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	480.02	J/mol×K	731.1	Joback Method
η	0.00	Pa×s	731.1	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H12O3/c1-18-15(17)13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10H,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).