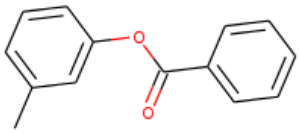
Benzoic acid, 3-methylphenyl ester

InChI: InChI=1S/C14H12O2/c1-11-6-5-9-13(10-11)16-14(15)12-7-3-2-4-8-12/h2-10H,1H3
InChI Key: XYKFCIJKMCQULO-UHFFFAOYSA-N
Formula: C14H12O2
SMILES: Cc1cccc(OC(=O)c2ccccc2)c1
Molecular Weight: 212.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	48.27	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-115.50	kJ/mol	Joback Method
$\Delta_{fus} H°$	22.50	kJ/mol	Joback Method
$\Delta_{vap} H°$	61.13	kJ/mol	Joback Method
$logP_{oct/wat}$	3.21		Crippen Method
P_c	2862.74	kPa	Joback Method
T_{boil}	654.35	K	Joback Method
T_c	898.02	K	Joback Method
T_{fus}	385.06	K	Joback Method
V_c	0.63	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	415.01	J/mol×K	654.35	Joback Method
η	0.00	Pa×s	654.35	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H12O2/c1-11-6-5-9-13(10-11)16-14(15)12-7-3-2-4-8-12/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).