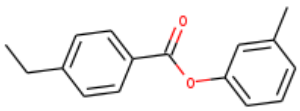
4-Ethylbenzoic acid, 3-methylphenyl ester

InChI: InChI=1S/C16H16O2/c1-3-13-7-9-14(10-8-13)16(17)18-15-6-4-5-12(2)11-15/h4-11H,3H2,1-2H3
InChI Key: HQCHUVGMZRKHRM-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CCc1ccc(C(=O)Oc2cccc(C)c2)cc1
Molecular Weight: 240.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	55.48	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-168.25	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.29	kJ/mol	Joback Method
$\Delta_{vap} H°$	66.24	kJ/mol	Joback Method
$logP_{oct/wat}$	3.78		Crippen Method
P_c	2320.31	kPa	Joback Method
T_{boil}	705.09	K	Joback Method
T_c	939.69	K	Joback Method
T_{fus}	420.12	K	Joback Method
V_c	0.74	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	517.05	J/mol×K	705.09	Joback Method
η	0.00	Pa×s	705.09	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H16O2/c1-3-13-7-9-14(10-8-13)16(17)18-15-6-4-5-12(2)11-15/h4-11H,3H2,1-2H3
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).