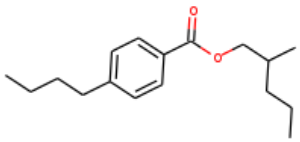
4-Butylbenzoic acid, 2-methylpentyl ester

InChI: InChI=1S/C17H26O2/c1-4-6-8-15-9-11-16(12-10-15)17(18)19-13-14(3)7-5-2/h9-12,14H,4-8,13H2,1-3H3
InChI Key: FAXLCUOSVAHYMS-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCc1ccc(C(=O)OCC(C)CCC)cc1
Molecular Weight: 262.39



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-41.32	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-419.23	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.70	kJ/mol	Joback Method
$\Delta_{vap} H°$	65.14	kJ/mol	Joback Method
$logP_{oct/wat}$	4.62		Crippen Method
P_c	1625.91	kPa	Joback Method
T_{boil}	695.87	K	Joback Method
T_c	893.18	K	Joback Method
T_{fus}	377.45	K	Joback Method
V_c	0.90	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	655.09	J/mol×K	695.87	Joback Method
η	0.00	Pa×s	695.87	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H26O2/c1-4-6-8-15-9-11-16(12-10-15)17(18)19-13-14(3)7-5-2/h9-12,14H,4-8,13H2,1-3H3
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).