

4-Butylbenzoic acid, 2-methylpentyl ester

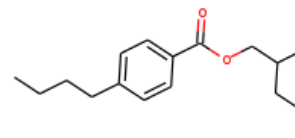
InChI: InChI=1S/C17H26O2/c1-4-6-8-15-9-11-16(12-10-15)17(18)19-13-14(3)7-5-2/h9-12,14H,4-8,13H2,1-3H3

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
$\Delta_f G^\circ$	-41.32	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-419.23	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.70	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	65.14	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	655.09	J/mol×K	695.87	Joback Method
η	0.00	Paxs	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](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/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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