

4-Butylbenzoic acid, pent-2-en-4-ynyl ester

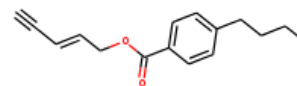
InChI: InChI=1S/C16H18O2/c1-3-5-7-13-18-16(17)15-11-9-14(10-12-15)8-6-4-2/h1,5,7,9-12H,4,6,8,13H2,2H3/b7-5+

InChI Key: JKKNXQJVFQVSHN-FNORWQNLSA-N

Formula: C16H18O2

SMILES: C#CC=CCOC(=O)c1ccc(CCCC)cc1

Molecular Weight: 242.31



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	255.99	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	15.81	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.81	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	63.12	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.38		Crippen Method
P_c	2081.22	kPa	Joback Method
T_{boil}	667.71	K	Joback Method
T_c	882.93	K	Joback Method
T_{fus}	423.07	K	Joback Method
V_c	0.79	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	530.93	J/mol×K	667.71	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H18O2/c1-3-5-7-13-18-16\(17\)15-11-9-14\(10-12-15\)8-6-4-2/h1,5,7,9-12H,4,6,8,13H2,2H3/b7-5+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H18O2/c1-3-5-7-13-18-16(17)15-11-9-14(10-12-15)8-6-4-2/h1,5,7,9-12H,4,6,8,13H2,2H3/b7-5+)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

$\Delta_f G^\circ$: 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).

$\log P_{oct/wat}$: 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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