

4-Butylbenzoic acid, heptadecyl ester

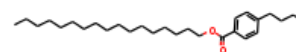
InChI: InChI=1S/C28H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-25-30-28(29)27-23-21-26(22-24-27)20-6-4-2/h21-24H,3-20,25H2,1-2H3

InChI Key: VRWCPSOWOJJUQU-UHFFFAOYSA-N

Formula: C28H48O2

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccc(CCCC)cc1

Molecular Weight: 416.68



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	53.74	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-640.99	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	64.72	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	90.02	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.06		Crippen Method
P_c	796.18	kPa	Joback Method
T_{boil}	947.99	K	Joback Method
T_c	1161.23	K	Joback Method
T_{fus}	516.42	K	Joback Method
V_c	1.52	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1320.05	J/mol×K	947.99	Joback Method
η	0.00	Paxs	947.99	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-25-30-28\(29\)27-23-21-26\(22-24-27\)20-6-4-2/h21-24H,3-20,25H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-25-30-28(29)27-23-21-26(22-24-27)20-6-4-2/h21-24H,3-20,25H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

η : Dynamic viscosity (Pa×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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