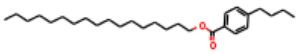
4-Butylbenzoic acid, heptadecyl ester

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
$\Delta_f G°$	53.74	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-640.99	kJ/mol	Joback Method
$\Delta_{fus} H°$	64.72	kJ/mol	Joback Method
$\Delta_{vap} H°$	90.02	kJ/mol	Joback Method
$logP_{oct/wat}$	9.057		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	1.520	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1320.05	J/mol×K	947.99	Joback Method
η	0.0000242	Pa×s	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
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).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).