

# Isophthalic acid, butyl hex-3-yl ester

**Other names:** Isophthalic acid, butyl hex-3-yl ester.

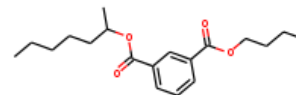
**InChI:** InChI=1S/C19H28O4/c1-4-6-8-10-15(3)23-19(21)17-12-9-11-16(14-17)18(20)22-13-7-5-2/h9,11-12,14-15H,4-8,10,13H2,1-3H3

**InChI Key:** ILRGMDONVIOSJD-UHFFFAOYSA-N

**Formula:** C<sub>19</sub>H<sub>28</sub>O<sub>4</sub>

**SMILES:** CCCCC(C)OC(=O)c1cccc(C(=O)OCCCC)c1

**Molecular Weight:** 320.42



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-258.40	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-705.31	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	40.67	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.75	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.77		Crippen Method
$P_c$	1450.14	kPa	Joback Method
$T_{\text{boil}}$	817.92	K	Joback Method
$T_c$	1019.49	K	Joback Method
$T_{\text{fus}}$	472.15	K	Joback Method
$V_c$	1.03	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	819.59	J/mol×K	817.92	Joback Method
$\eta$	0.00	Paxs	817.92	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-4-6-8-10-15\(3\)23-19\(21\)17-12-9-11-16\(14-17\)18\(20\)22-13-7-5-2/h9,11-12,14-15H,4-8,10,13H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-4-6-8-10-15(3)23-19(21)17-12-9-11-16(14-17)18(20)22-13-7-5-2/h9,11-12,14-15H,4-8,10,13H2,1-3H3)

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

## Legend

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

$\eta$ : 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 (m<sup>3</sup>/kg-mol).

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