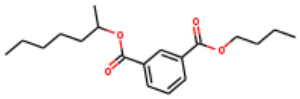
Isophthalic acid, butyl hex-3-yl ester

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: C19H28O4
SMILES: CCCCCC(C)OC(=O)c1cccc(C(=O)OCCCC)c1
Molecular Weight: 320.42



Physical Properties

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

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	819.59	J/mol×K	817.92	Joback Method
η	0.00	Pa×s	817.92	Joback Method

Sources

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).