

Isophthalic acid, isohexyl pent-4-enyl ester

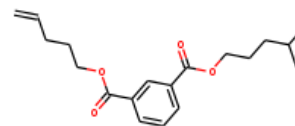
InChI: InChI=1S/C19H26O4/c1-4-5-6-12-22-18(20)16-10-7-11-17(14-16)19(21)23-13-8-9-15(2)3/h4,7,10-11,14-15H,1,5-6,8-9,12-13H2,2-3H3

InChI Key: MGNWETZBCZH XIQ-UHFFFAOYSA-N

Formula: C₁₉H₂₆O₄

SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Molecular Weight: 318.41



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-170.56	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-579.88	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.39	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.08	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.40		Crippen Method
P_c	1497.67	kPa	Joback Method
T_{boil}	814.60	K	Joback Method
T_c	1018.14	K	Joback Method
T_{fus}	470.39	K	Joback Method
V_c	1.01	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	792.85	J/mol×K	814.6	Joback Method
η	0.00	Paxs	814.6	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H26O4/c1-4-5-6-12-22-18\(20\)16-10-7-11-17\(14-16\)19\(21\)23-13-8-9-15\(2\)3/h4,7,10-11,14-15H,1,5-6,8-9,12-13H2,2-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H26O4/c1-4-5-6-12-22-18(20)16-10-7-11-17(14-16)19(21)23-13-8-9-15(2)3/h4,7,10-11,14-15H,1,5-6,8-9,12-13H2,2-3H3)

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

Legend

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

η : 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 (m³/kg-mol).

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