

Succinic acid, butyl 4-iodobenzyl ester

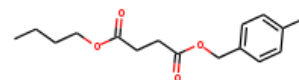
InChI: InChI=1S/C15H19IO4/c1-2-3-10-19-14(17)8-9-15(18)20-11-12-4-6-13(16)7-5-12/h4-7H,2-3,8-11H2,1H3

InChI Key: UAHQVWKOFFVIGC-UHFFFAOYSA-N

Formula: C15H19IO4

SMILES: CCCOC(=O)CCC(=O)OCc1ccc(I)cc1

Molecular Weight: 390.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-231.52	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-540.60	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	38.24	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	79.61	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.46		Crippen Method
P_c	1937.24	kPa	Joback Method
T_{boil}	819.98	K	Joback Method
T_c	1044.02	K	Joback Method
T_{fus}	500.13	K	Joback Method
V_c	0.90	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	642.89	J/mol×K	819.98	Joback Method
η	0.00	Paxs	819.98	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19IO4/c1-2-3-10-19-14\(17\)8-9-15\(18\)20-11-12-4-6-13\(16\)7-5-12/h4-7H,2-3,8-11H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19IO4/c1-2-3-10-19-14(17)8-9-15(18)20-11-12-4-6-13(16)7-5-12/h4-7H,2-3,8-11H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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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