

Succinic acid, heptyl 3-methylbenzyl ester

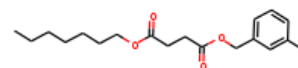
InChI: InChI=1S/C19H28O4/c1-3-4-5-6-7-13-22-18(20)11-12-19(21)23-15-17-10-8-9-16(2)14-17/h8-10,14H,3-7,11-13,15H2,1-2H3

InChI Key: KZSFYQISTWLZTM-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCCCCCOC(=O)CCC(=O)OCc1cccc(C)c1

Molecular Weight: 320.42



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-255.96	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-700.03	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	44.19	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	79.14	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.33		Crippen Method
P_c	1441.35	kPa	Joback Method
T_{boil}	818.36	K	Joback Method
T_c	1017.87	K	Joback Method
T_{fus}	487.15	K	Joback Method
V_c	1.04	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	819.06	J/mol×K	818.36	Joback Method
η	0.00	Paxs	818.36	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-3-4-5-6-7-13-22-18\(20\)11-12-19\(21\)23-15-17-10-8-9-16\(2\)14-17/h8-10,14H,3-7,11-13,15H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-3-4-5-6-7-13-22-18(20)11-12-19(21)23-15-17-10-8-9-16(2)14-17/h8-10,14H,3-7,11-13,15H2,1-2H3)

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

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol \times K).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: 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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