

Sebacic acid, isobutyl nonyl ester

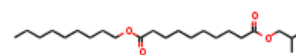
InChI: InChI=1S/C23H44O4/c1-4-5-6-7-10-13-16-19-26-22(24)17-14-11-8-9-12-15-18-23(25)27-20-21(2)3/h21H,4-20H2,1-3H3

InChI Key: RERNDEIBYJZPEF-UHFFFAOYSA-N

Formula: C23H44O4

SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)C

Molecular Weight: 384.59



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-327.50	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1012.93	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	57.38	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	84.72	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.60		Crippen Method
P_c	903.97	kPa	Joback Method
T_{boil}	877.78	K	Joback Method
T_c	1074.72	K	Joback Method
T_{fus}	478.29	K	Joback Method
V_c	1.37	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1154.96	J/mol×K	877.78	Joback Method
η	0.00	Paxs	877.78	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H44O4/c1-4-5-6-7-10-13-16-19-26-22\(24\)17-14-11-8-9-12-15-18-23\(25\)27-20-21\(2\)3/h21H,4-20H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H44O4/c1-4-5-6-7-10-13-16-19-26-22(24)17-14-11-8-9-12-15-18-23(25)27-20-21(2)3/h21H,4-20H2,1-3H3)

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

Legend

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

η : Dynamic viscosity (Pa×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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