

Sebacic acid, isobutyl 4-octyl ester

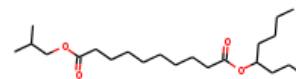
InChI: InChI=1S/C22H42O4/c1-5-7-15-20(14-6-2)26-22(24)17-13-11-9-8-10-12-16-21(23)25-18-19(3)4/h19-20H,5-18H2,1-4H3

InChI Key: FVMYRMOZJVKLDW-UHFFFAOYSA-N

Formula: C22H42O4

SMILES: CCCCC(CCC)OC(=O)CCCCCCCCC(=O)OCC(C)C

Molecular Weight: 370.57



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-338.36	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-997.57	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	51.26	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	82.10	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.209		Crippen Method
P_c	963.27	kPa	Joback Method
T_{boil}	854.46	K	Joback Method
T_c	1046.57	K	Joback Method
T_{fus}	452.02	K	Joback Method
V_c	1.304	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1092.98	J/mol×K	854.46	Joback Method
η	0.0000333	Paxs	854.46	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H42O4/c1-5-7-15-20\(14-6-2\)26-22\(24\)17-13-11-9-8-10-12-16-21\(23\)25-18-19\(3\)4/h19-20H,5-18H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H42O4/c1-5-7-15-20(14-6-2)26-22(24)17-13-11-9-8-10-12-16-21(23)25-18-19(3)4/h19-20H,5-18H2,1-4H3)

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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