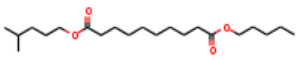
# Sebacic acid, isohexyl pentyl ester

**InChI**: InChI=1S/C21H40O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19(2)3/h19H,4-18H2,1-3H3
**InChI Key**: PXCSJSVAODQQQL-UHFFFAOYSA-N
**Formula**: C21H40O4
**SMILES**: CCCCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
**Molecular Weight**: 356.54



## Physical Properties

| Property | Value | Unit | Source |
|---|---|---|---|
| $\Delta_f G°$ | -344.34 | kJ/mol | Joback Method |
| $\Delta_f H°_{gas}$ | -971.65 | kJ/mol | Joback Method |
| $\Delta_{fus} H°$ | 52.20 | kJ/mol | Joback Method |
| $\Delta_{vap} H°$ | 80.26 | kJ/mol | Joback Method |
| $logP_{oct/wat}$ | 5.82 | | Crippen Method |
| $P_c$ | 1018.13 | kPa | Joback Method |
| $T_{boil}$ | 832.02 | K | Joback Method |
| $T_c$ | 1019.80 | K | Joback Method |
| $T_{fus}$ | 455.75 | K | Joback Method |
| $V_c$ | 1.25 | $m^3$/kg-mol | Joback Method |

## Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|---|---|---|---|---|
| $C_{p,gas}$ | 1030.73 | J/mol×K | 832.02 | Joback Method |
| η | 0.00 | Pa×s | 832.02 | Joback Method |

## Sources

**Joback Method**: https://en.wikipedia.org/wiki/Joback_method
**NIST Webbook**: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H40O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19(2)3/h19H,4-18H2,1-3H3
**Crippen Method**: http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume ($m^3$/kg-mol).