

Sebacic acid, isohexyl pentyl ester

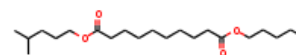
InChI: InChI=1S/C21H40O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19(2)3/h19H,4-18H2,1-3H3

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
$\Delta_f G^\circ$	-344.34	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-971.65	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	52.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.26	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.820		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	1.254	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1030.73	J/mol×K	832.02	Joback Method
η	0.0000422	Paxs	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](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/ci9903071>

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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