

# Decanedioic acid, bis(2-ethylhexyl) ester

## Other names:

1-Hexanol, 2-ethyl-, sebacate  
2-Ethylhexyl sebacate  
BEHS  
Bis(2-ethylhexyl) ester, decanedionic acid  
Bis(2-ethylhexyl) ester, sebacic acid  
Bis(ethylhexyl) sebacate  
Bis-(2-ethylhexyl)ester kyseliny sebakove  
Bisoflex  
Bisoflex DOS  
DOS  
Decanedioic acid, 1,10-bis(2-ethylhexyl) ester  
Decanedioic acid, di-(2-ethylhexyl) ester  
Di(2-ethylhexyl) sebacate  
Dioctyl sebacate  
Edenol 888  
Edenor DEHS  
Ergoplast SDO  
Ergoplast SNO  
Monoplex DOS  
NSC 68878  
Octoil s  
Plasthall DOS  
Plexol  
Plexol 201  
Plexol 201J  
Px 438  
Reolube dos  
Reomol DDS  
Sansocizer DOS  
Sebacic acid di(2-ethylhexyl) ester  
Sebacic acid, dioctyl ester-  
Stafllex dos  
Uniflex DOS  
bis(2-ethylhexyl) decanedioate  
bis(2-ethylhexyl) sebacate  
di-(2-ethylhexyl) sebacate  
sebacic acid, bis(2-ethylhexyl) ester

## Inchi:

InChI=1S/C26H50O4/c1-5-9-17-23(7-3)21-29-25(27)19-15-13-11-12-14-16-20-26(28)30-

## InchiKey:

VJHINFRRDQUWOJ-UHFFFAOYSA-N

## Formula:

C<sub>26</sub>H<sub>50</sub>O<sub>4</sub>

**SMILES:** CCCCC(CC)COC(=O)CCCCCCCCC(=O)OCC(CC)CCCC  
**Mol. weight [g/mol]:** 426.67  
**CAS:** 122-62-3

## Physical Properties

Property code	Value	Unit	Source
gf	-304.68	kJ/mol	Joback Method
hf	-1080.13	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	945.98	K	Joback Method
tc	1162.69	K	Joback Method
tf	497.10	K	Joback Method
vc	1.528	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/molxK	945.98	Joback Method
cpg	1367.00	J/molxK	982.10	Joback Method
cpg	1386.38	J/molxK	1018.22	Joback Method
cpg	1404.14	J/molxK	1054.33	Joback Method
cpg	1420.33	J/molxK	1090.45	Joback Method
cpg	1435.00	J/molxK	1126.57	Joback Method
cpg	1448.19	J/molxK	1162.69	Joback Method
dvisc	0.0038430	Paxs	353.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0327700	Paxs	283.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0260100	Paxs	288.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0210000	Paxs	293.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0172100	Paxs	298.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0143200	Paxs	303.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0120700	Paxs	308.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0102800	Paxs	313.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0088450	Paxs	318.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0076790	Paxs	323.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0067270	Paxs	328.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0059390	Paxs	333.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0052750	Paxs	338.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0047190	Paxs	343.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0042480	Paxs	348.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0420400	Paxs	278.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0034940	Paxs	358.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0031690	Paxs	363.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0029020	Paxs	368.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0026610	Paxs	373.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0319500	Paxs	284.06	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0258400	Paxs	288.71	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0211400	Paxs	293.37	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0174200	Paxs	298.26	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0145500	Paxs	303.10	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0123700	Paxs	307.90	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa

dvisc	0.0036260	Paxs	358.09	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0090230	Paxs	318.26	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0078650	Paxs	323.17	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0068780	Paxs	328.26	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0060670	Paxs	333.20	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0054350	Paxs	338.16	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa

dvisc	0.0048830	Paxs	342.81	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0043800	Paxs	348.07	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0039870	Paxs	352.98	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
dvisc	0.0104000	Paxs	313.24	Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa
hvapt	114.90	kJ/mol	380.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.20	K	0.10	NIST Webbook
tbrp	529.20	K	0.70	NIST Webbook

Datasets

Molar heat capacity at constant pressure, J/K/mol

Temperature, K - Liquid	Pressure, kPa - Liquid	Molar heat capacity at constant pressure, J/K/mol - Liquid
293.15	100.00	810.30
293.15	10000.00	808.50
293.15	20000.00	805.60
293.15	30000.00	803.00
313.15	100.00	846.50
313.15	10000.00	843.50
313.15	20000.00	840.10
313.15	30000.00	838.40
333.15	100.00	878.10
333.15	10000.00	875.50
333.15	20000.00	873.40
333.15	30000.00	871.70
353.15	100.00	910.90
353.15	10000.00	909.70
353.15	20000.00	907.10
353.15	30000.00	906.30

Reference

<https://www.doi.org/10.1016/j.jct.2012.01.011>

Sources

An experimental setup for isobaric heat capacities for viscous fluids at high pressure: Squalane, bis(2-ethylhexyl) sebacate and bis(2-ethylhexyl) phthalate.

Joback Method:

McGowan Method:

Crippen Method:

Equilibrium Solubilities of Diisooctyl Sebacate in Supercritical Carbon Dioxide: Experimental density and viscosity measurements of the mixtures of Diisooctyl Sebacate with Squalane, Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa:

<https://www.doi.org/10.1016/j.jct.2012.01.011>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C122623&Units=SI>

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

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<https://www.doi.org/10.1021/acs.jced.5b00457>

<https://www.doi.org/10.1016/j.jct.2011.07.005>

<https://www.doi.org/10.1021/je4005245>

Legend



<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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