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-
Staflex 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: C26H50O4

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	1448.19	J/mol×K	1162.69	Joback Method
cpg	1345.96	J/mol×K	945.98	Joback Method
cpg	1367.00	J/mol×K	982.10	Joback Method
cpg	1386.38	J/mol×K	1018.22	Joback Method
cpg	1404.14	J/mol×K	1054.33	Joback Method
cpg	1420.33	J/mol×K	1090.45	Joback Method
cpg	1435.00	J/mol×K	1126.57	Joback Method
dvisc	0.0260100	Pa×s	288.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0420400	Pa×s	278.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0327700	Pa×s	283.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0039870	Pa×s	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	0.0210000	Pa×s	293.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0172100	Pa×s	298.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0143200	Pa×s	303.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0120700	Pa×s	308.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0102800	Pa×s	313.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0088450	Pa×s	318.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0076790	Pa×s	323.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0067270	Pa×s	328.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0059390	Pa×s	333.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0052750	Pa×s	338.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0047190	Pa×s	343.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0042480	Pa×s	348.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0038430	Pa×s	353.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0034940	Pa×s	358.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0031690	Pa×s	363.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0029020	Pa×s	368.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure

dvisc	0.0026610	Pa×s	373.15	Experimental density and viscosity measurements of di(2ethylhexyl)sebacate at high pressure
dvisc	0.0319500	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	0.0104000	Pa×s	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	
dvisc	0.0090230	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	Pa×s	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	0.0036260	Pa×s	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
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:	https://www.doi.org/10.1016/j.jct.2012.01.011
Equilibrium Solubilities of Diisooctyl Sebacate in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.5b00457
Modified Wilson Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental density and viscosity measurements of Di(2-ethylhexyl) sebacate at high pressures:	https://www.doi.org/10.1016/j.jct.2011.07.005
Measurements of the Viscosity of Bis(2-ethylhexyl) Sebacate, Squalane, and Bis(2-ethylhexyl) Phthalate between (283 and 363) K at 0.1 MPa:	https://www.doi.org/10.1021/je4005245
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122623&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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