Decanedioic acid, diethyl ester

Other names:	Bisoflex DES
	Decanedioic acid, 1,10-diethyl ester
	Diethyl 1,10-decanedioate
	Diethyl decanedioate
	Diethyl sebacate
	Ethyl sebacate
	NSC 8911
	Sebacic acid, diethyl ester
Inchi:	InChI=1S/C14H26O4/c1-3-17-13(15)11-9-7-5-6-8-10-12-14(16)18-4-2/h3-12H2,1-2H3
InchiKey:	ONKUXPIBXRRIDU-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CCOC(=O)CCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	258.35
CAS:	110-40-7

Physical Properties

Property code	Value	Unit	Source
gf	-400.84	kJ/mol	Joback Method
hf	-821.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-3.51		Aqueous Solubility Prediction Method
logp	3.233		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1746.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1746.00		NIST Webbook
ripol	2272.00		NIST Webbook
tb	585.20	K	NIST Webbook

tc	740.00	K	Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters
tf	276.65	K	Aqueous Solubility Prediction Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.29	J/mol×K	848.26	Joback Method
cpg	622.19	J/mol×K	672.30	Joback Method
cpg	637.83	J/mol×K	701.63	Joback Method
cpg	652.75	J/mol×K	730.95	Joback Method
cpg	666.95	J/mol×K	760.28	Joback Method
cpg	680.44	J/mol×K	789.61	Joback Method
cpg	693.22	J/mol×K	818.93	Joback Method
dvisc	0.0001198	Pa×s	672.30	Joback Method
dvisc	0.0014859	Pa×s	391.86	Joback Method
dvisc	0.0007810	Pa×s	438.60	Joback Method
dvisc	0.0004646	Pa×s	485.34	Joback Method
dvisc	0.0003028	Pa×s	532.08	Joback Method
dvisc	0.0002115	Pa×s	578.82	Joback Method
dvisc	0.0001558	Pa×s	625.56	Joback Method
hvapt	74.10	kJ/mol	488.50	NIST Webbook
rhol	959.18	kg/m3	298.20	Modeling phase equilibria of ternary systems (water + formic acid + ester or alcohol) through UNIFAC-original, SERLAS, NRTL, NRTL-modified, and three-suffix Margules: Parameter estimation using genetic algorithm

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74579e+01
Coeff. B	-7.11540e+03
Coeff. C	-3.10220e+01
Temperature range (K), min.	445.42
Temperature range (K), max.	616.82

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Comparison of Extractability of Oxalic Acid from Dilute Aqueous Solutions Using Dioctylamine and Trioctylphosphine Oxide:	https://www.doi.org/10.1021/acs.jced.8b01155
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Modeling phase equilibria of ternary systems (water + formic acid + ester or alcohol) through UNIFAC-original, SERLAS, NRTL, NRTL-modified, and three-suffix Margules: Parameter estimation using genetic algorithm:	https://www.doi.org/10.1016/j.fluid.2016.08.041
Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters:	https://www.doi.org/10.1016/j.jct.2017.09.004
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110407&Units=SI

Legend

cpg:	Ideal gas 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
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume