Decanedioic acid, dibutyl ester

Other names:	Bis(n-butyl) sebacate
	Butyl sebacate
	Decanedioic acid, 1,10-dibutyl ester
	Di(n-butyl) sebacate
	Dibutyl decanedioate
	Dibutyl sebacate
	Dibutyl sebacinate
	Dibutylester kyseliny sebakove
	Kodaflex DBS
	Monoplex dbs
	NSC 3893
	PX 404
	Plasthall DBS
	Polycizer DBS
	Reomol DBS
	Sebacic acid, dibutyl ester
	Staflex DBS
	Uniflex DBS
	decandioic acid, dibutyl ester
	n-Butyl sebacate
Inchi:	InChI=1S/C18H34O4/c1-3-5-15-21-17(19)13-11-9-7-8-10-12-14-18(20)22-16-6-4-2/h3-16
InchiKey:	PYGXAGIECVVIOZ-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCOC(=O)CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	314.46
CAS:	109-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-367.16	kJ/mol	Joback Method
hf	-904.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	91.80 ± 3.20	kJ/mol	NIST Webbook
log10ws	-3.72		Aqueous Solubility Prediction Method
log10ws	-3.90		Estimated Solubility Method

logp	4.794		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2180.10		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	763.82	K	Joback Method
tc	942.53	K	Joback Method
tf	262.65	K	Aqueous Solubility Prediction Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.49	J/mol×K	763.82	Joback Method
cpg	866.90	J/mol×K	793.61	Joback Method
cpg	883.40	J/mol×K	823.39	Joback Method
cpg	898.98	J/mol×K	853.18	Joback Method
cpg	913.68	J/mol×K	882.96	Joback Method
cpg	927.49	J/mol×K	912.75	Joback Method
cpg	940.44	J/mol×K	942.53	Joback Method
cpl	619.00	J/mol×K	312.00	NIST Webbook
dvisc	0.0000707	Pa×s	763.82	Joback Method
dvisc	0.0005169	Pa×s	491.42	Joback Method
dvisc	0.0010365	Pa×s	436.94	Joback Method
dvisc	0.0001878	Pa×s	600.38	Joback Method
dvisc	0.0001284	Pa×s	654.86	Joback Method
dvisc	0.0000931	Pa×s	709.34	Joback Method
dvisc	0.0002962	Pa×s	545.90	Joback Method
hvapt	106.40	kJ/mol	500.00	NIST Webbook
hvapt	87.60	kJ/mol	466.00	NIST Webbook
hvapt	88.10	kJ/mol	327.00	NIST Webbook
hvapt	94.30	kJ/mol	460.50	NIST Webbook

rfi	1.44200		298.10	Isobaric vapor liquid equilibria of the binary system: Maleic anhydride + di-n-butylsebacate at 2.67, 5.33 and 8.00 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47404e+01
Coeff. B	-5.63216e+03
Coeff. C	-9.08550e+01
Temperature range (K), min.	480.55
Temperature range (K), max.	688.18

Sources

Isobaric vapor liquid equilibria of the binary system: Maleic anhydride + di-n-butylsebacate at 2.67, 5.33 and 8.00 kPa:	https://www.doi.org/10.1016/j.fluid.2008.08.001
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume