

Butanedioic acid, dibutyl ester

Other names:	B-9 Butanedioic acid, 1,4-dibutyl ester Butyl butanedioate DNBS Di-n-butylester kyseliny jantarove Dibutyl butanedioate ENT 666 NSC 1502 Succinic acid di-n-butyl ester Tabatrex Tabutrex di-n-butyl succinate dibutyl succinate succinic acid, dibutyl ester
Inchi:	InChI=1S/C12H22O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h3-10H2,1-2H3
InchiKey:	YUXIBTJKHLUKBD-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCCOC(=O)CCC(=O)OCCCC
Mol. weight [g/mol]:	230.30
CAS:	141-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-417.68	kJ/mol	Joback Method
hf	-780.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.453		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1528.00		NIST Webbook

rinpol	1528.00		NIST Webbook
rinpol	1534.00		NIST Webbook
ripol	2000.00		NIST Webbook
sl	548.44	J/mol×K	NIST Webbook
tb	547.70 ± 1.00	K	NIST Webbook
tb	408.00 ± 6.00	K	NIST Webbook
tc	803.91	K	Joback Method
tf	369.32	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.78	J/mol×K	803.91	Joback Method
cpg	530.51	J/mol×K	656.10	Joback Method
cpg	544.42	J/mol×K	685.66	Joback Method
cpg	557.71	J/mol×K	715.23	Joback Method
cpg	570.37	J/mol×K	744.79	Joback Method
cpg	582.39	J/mol×K	774.35	Joback Method
cpg	515.96	J/mol×K	626.54	Joback Method
cpl	436.24	J/mol×K	298.15	NIST Webbook
dvisc	0.0001965	Pa×s	583.67	Joback Method
dvisc	0.0002641	Pa×s	540.80	Joback Method
dvisc	0.0003735	Pa×s	497.93	Joback Method
dvisc	0.0005638	Pa×s	455.06	Joback Method
dvisc	0.0009273	Pa×s	412.19	Joback Method
dvisc	0.0001522	Pa×s	626.54	Joback Method
dvisc	0.0017118	Pa×s	369.32	Joback Method
hfust	29.21	kJ/mol	244.13	NIST Webbook
hfust	29.21	kJ/mol	244.10	NIST Webbook
hfust	29.21	kJ/mol	244.10	NIST Webbook
pvap	2.05e-03	kPa	318.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	8.77e-03	kPa	335.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.01	kPa	338.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	3.25e-03	kPa	323.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	343.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	346.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	349.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	352.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.04	kPa	355.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.05	kPa	358.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	3.83e-03	kPa	325.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	7.43e-03	kPa	333.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	5.77e-03	kPa	330.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	4.89e-03	kPa	328.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	1.32e-03	kPa	313.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	1.70e-03	kPa	316.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	2.48e-03	kPa	320.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.01	kPa	340.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
rhof	938.70	kg/m3	333.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhof	947.80	kg/m3	323.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhof	957.00	kg/m3	313.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhof	966.20	kg/m3	303.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhof	975.30	kg/m3	293.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
sfust	119.60	J/mol×K	244.13	NIST Webbook

Sources

Crippen Method:

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

Solubilities and thermodynamic properties of SO2 in five biobased solvents:

<https://www.doi.org/10.1016/j.jct.2015.09.017>

Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetrical Linear n-Alkyl Esters of Dicarboxylic Acids: McGowan Method:

<https://www.doi.org/10.1021/je100231g>

https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C141037&Units=SI>

Phase Behavior of Binary Mixtures Containing Succinic Acid or Its Esters: Solubilities of Carbon Dioxide in Five Bio-based Solvents: Crippen Method:

<https://www.doi.org/10.1021/acs.jced.7b00005>

<https://www.doi.org/10.1021/je500812s>

https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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