2-Butenedioic acid (Z)-, dibutyl ester

Other names:	2-Butenedioic acid (2Z)-, 1,4-dibutyl ester
	2-Butenedioic acid (2Z)-, dibutyl ester
	2-Butenedioic acid, dibutyl ester, cis-
	Bibutyl maleate
	Bisomer DBM
	Butyl maleate
	DBM
	Dibutyl (2z)-2-butenedioate
	Dibutyl maleate
	Dibutylester kyseliny maleinove
	Maleic acid, dibutyl ester
	Octomer DBM
	PX-504
	RC Comonomer DBM
	Staflex DBM
	cis-butenedioic acid, dibutyl ester
	di-n-Butyl maleate
	dibutyl cis-butendioate
	dibutyl maleinate
Inchi:	InChI=1S/C12H20O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h7-8H,3-6,9-10H2,1-2H3
InchiKey:	JBSLOWBPDRZSMB-FPLPWBNLSA-N
Formula:	C12H20O4
SMILES:	CCCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]:	228.28
CAS:	105-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-337.46	kJ/mol	Joback Method
hf	-663.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1505.00		NIST Webbook

rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
tb	553.40 ± 0.50	K	NIST Webbook
tb	554.20	K	NIST Webbook
tc	814.25	K	Joback Method
tf	364.24	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.75	J/mol×K	814.25	Joback Method
cpg	495.03	J/mol×K	630.70	Joback Method
cpg	509.10	J/mol×K	661.29	Joback Method
cpg	522.51	J/mol×K	691.88	Joback Method
cpg	535.27	J/mol×K	722.48	Joback Method
cpg	547.40	J/mol×K	753.07	Joback Method
cpg	558.89	J/mol×K	783.66	Joback Method
dvisc	0.0001303	Pa×s	630.70	Joback Method
dvisc	0.0015837	Pa×s	364.24	Joback Method
dvisc	0.0008330	Pa×s	408.65	Joback Method
dvisc	0.0004970	Pa×s	453.06	Joback Method
dvisc	0.0003252	Pa×s	497.47	Joback Method
dvisc	0.0002281	Pa×s	541.88	Joback Method
dvisc	0.0001688	Pa×s	586.29	Joback Method
hvapt	41.10	kJ/mol	402.50	NIST Webbook
rhol	990.10	kg/m3	293.15	Correlation of Experimental Liquid Liquid Equilibrium Data for Ternary Systems Using NRTL and GMDH-Type Neural Network

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78368e+01
Coeff. B	-7.64066e+03
Coeff. C	2.38300e+01
Temperature range (K), min.	411.56
Temperature range (K), max.	586.19

Sources

Correlation of Experimental Liquid Liquid Equilibrium Data for Ternary Systems Using NRTL and GMDH-Type Neural Network:	https://www.doi.org/10.1021/acs.jced.6b00985
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105760&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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