Carbonic acid, dibutyl ester

Other names:	Carbonic acid, di-n-butyl ester
	Di-n-butyl carbonate
	dibutyl carbonate
	n-C4H9OC(O)OC4H9-n
	n-butyl carbonate
Inchi:	InChI=1S/C9H18O3/c1-3-5-7-11-9(10)12-8-6-4-2/h3-8H2,1-2H3
InchiKey:	QLVWOKQMDLQXNN-UHFFFAOYSA-N
Formula:	C9H18O3
SMILES:	CCCCOC(=O)OCCCC
Mol. weight [g/mol]:	174.24
CAS:	542-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-314.02	kJ/mol	Joback Method
hf	-606.11	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	62.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	2.740		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	481.00 ± 0.40	K	NIST Webbook
tb	480.60 ± 0.60	K	NIST Webbook
tc	677.20	K	Joback Method
tf	285.58	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.03	J/mol×K	504.03	Joback Method
cpg	361.09	J/mol×K	532.89	Joback Method
cpg	373.72	J/mol×K	561.75	Joback Method

cpg	385.91	J/mol×K	590.62	Joback Method
cpg	397.66	J/mol×K	619.48	Joback Method
cpg	408.97	J/mol×K	648.34	Joback Method
cpg	419.82	J/mol×K	677.20	Joback Method
dvisc	0.0024200	Pa×s	285.58	Joback Method
dvisc	0.0012601	Pa×s	321.99	Joback Method
dvisc	0.0007491	Pa×s	358.40	Joback Method
dvisc	0.0004902	Pa×s	394.81	Joback Method
dvisc	0.0003446	Pa×s	431.21	Joback Method
dvisc	0.0002559	Pa×s	467.62	Joback Method
dvisc	0.0001984	Pa×s	504.03	Joback Method
pvap	0.03	kPa	299.80	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.01	kPa	290.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.02	kPa	292.90	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.02	kPa	296.80	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	8.56e-03	kPa	287.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.03	kPa	300.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.03	kPa	302.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.03	kPa	303.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	0.04	kPa	305.00	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates

pvap	0.04	kPa	306.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.05	kPa	307.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.06	kPa	308.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.06	kPa	311.00	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.08	kPa	313.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.09	kPa	315.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.11	kPa	317.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.14	kPa	320.70	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.15	kPa	323.30	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.18	kPa	324.90	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.20	kPa	326.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	
pvap	0.24	kPa	329.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates	

rhol	925.17	kg/m3	298.15	Isobaric Vapor Liquid Equilibrium for Two Binary Systems (Methanol + Dibutyl Carbonate) and (n-Butanol + Dibutyl Carbonate) at p = 40.0, 70.0, and 100.0 kPa

Sources

Isobaric Vapor Liquid Equilibrium for Two Binary Systems (Methanol + Dibutyl Carbonate) and (n-Butanol + Dibutyl Carbonate) at p = 40.0, 70.0, and 100.0 kPa:	https://www.doi.org/10.1021/acs.jced.6b00517
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=C542529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates:	https://www.doi.org/10.1016/j.jct.2008.02.012

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