Pentanedioic acid, dibutyl ester

Other names:	Glutaric acid, dibutyl ester
	dibutyl glutarate
	dibutyl pentanedioate
Inchi:	InChI=1S/C13H24O4/c1-3-5-10-16-12(14)8-7-9-13(15)17-11-6-4-2/h3-11H2,1-2H3
InchiKey:	ISXDVFNOXYQPIA-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCCCOC(=O)CCCC(=O)OCCCC
Mol. weight [g/mol]:	244.33
CAS:	6624-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-409.26	kJ/mol	Joback Method
hf	-801.25	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.843		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1627.00		NIST Webbook
ripol	2014.00		NIST Webbook
tb	649.42	K	Joback Method
tc	825.90	K	Joback Method
tf	380.59	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	649.00	J/mol×K	825.90	Joback Method
cpg	583.50	J/mol×K	678.83	Joback Method
cpg	597.94	J/mol×K	708.25	Joback Method
cpg	611.72	J/mol×K	737.66	Joback Method
cpg	624.81	J/mol×K	767.07	Joback Method
cpg	637.24	J/mol×K	796.48	Joback Method
cpg	568.37	J/mol×K	649.42	Joback Method
dvisc	0.0001754	Pa×s	604.62	Joback Method
dvisc	0.0002370	Pa×s	559.81	Joback Method
dvisc	0.0003373	Pa×s	515.00	Joback Method
dvisc	0.0005134	Pa×s	470.20	Joback Method
dvisc	0.0008539	Pa×s	425.40	Joback Method
dvisc	0.0001354	Pa×s	649.42	Joback Method
dvisc	0.0016009	Pa×s	380.59	Joback Method
pvap	1.79e-03	kPa	328.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	1.73e-03	kPa	328.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	2.10e-03	kPa	330.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	2.29e-03	kPa	331.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	2.73e-03	kPa	333.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	3.06e-03	kPa	334.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	2.98e-03	kPa	334.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	1.45e-03	kPa	326.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	4.04e-03	kPa	338.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	4.75e-03	kPa	340.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	6.00e-03	kPa	343.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	7.82e-03	kPa	346.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	9.73e-03	kPa	349.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.01	kPa	350.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.01	kPa	352.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.01	kPa	354.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	357.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.02	kPa	360.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	363.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.03	kPa	366.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.04	kPa	369.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	1.32e-03	kPa	325.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	1.13e-03	kPa	323.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	1.14e-03	kPa	323.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	1.03e-03	kPa	322.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	7.00e-04	kPa	318.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	6.40e-04	kPa	317.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	3.75e-03	kPa	337.60	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6624573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je100231g
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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