Pentanoic acid, butyl ester

Other names:	Butyl pentanoate
	Butyl valerate
	Butyl valerianate
	N-BUTYL VALERATE
	Valeric acid, butyl ester
	n-Butyl pentanoate
	n-Butyl pentenoate
Inchi:	InChI=1S/C9H18O2/c1-3-5-7-9(10)11-8-6-4-2/h3-8H2,1-2H3
InchiKey:	OKJADYKTJJGKDX-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCOC(=O)CCCC
Mol. weight [g/mol]:	158.24
CAS:	591-68-4

Physical Properties

Property code	Value	Unit	Source
chl	-5500.70 ± 1.70	kJ/mol	NIST Webbook
gf	-209.02	kJ/mol	Joback Method
hf	-560.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-613.00 ± 2.00	kJ/mol	NIST Webbook
hfus	21.85	kJ/mol	Joback Method
hvap	53.00 ± 1.00	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1074.00		NIST Webbook
ripol	1314.00		NIST Webbook

ripol	1306.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1336.00		NIST Webbook
tb	459.00 ± 2.00	K	NIST Webbook
tb	460.00 ± 3.00	K	NIST Webbook
tc	655.29	K	Joback Method
tf	263.35	K	Joback Method
tt	189.37 ± 0.02	K	NIST Webbook
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	481.61	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	395.29	J/mol×K	655.29	Joback Method
dvisc	0.0033103	Pa×s	263.35	Joback Method
dvisc	0.0016384	Pa×s	299.73	Joback Method
dvisc	0.0009442	Pa×s	336.10	Joback Method
dvisc	0.0006060	Pa×s	372.48	Joback Method
dvisc	0.0004209	Pa×s	408.86	Joback Method
dvisc	0.0003103	Pa×s	445.23	Joback Method
dvisc	0.0002395	Pa×s	481.61	Joback Method
hvapt	41.00	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49789e+01
Coeff. B	-4.05166e+03
Coeff. C	-6.89330e+01

Temperature range (K), min.	344.72
Temperature range (K), max.	488.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57471e+01
Coeff. B	-8.44962e+03
Coeff. C	-7.04478e+00
Coeff. D	2.09353e-06
Temperature range (K), min.	180.35
Temperature range (K), max.	629.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1112
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1112.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591684&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/57-745-2/Pentanoic-acid-butyl-ester.pdf

Generated by Cheméo on 2024-10-12 08:00:56.098125045 +0000 UTC m=+3300918.735094293.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.