Butanoic acid, pentyl ester

Other names:	1-Pentyl butyrate
	AMYL N-BUTYRATE
	Amyl butanoate
	Amyl butyrate
	Butyric acid, pentyl ester
	PENTYL BUTANOATE
	Pentyl butyrate
	UN 2620
	n-Amyl butyrate
	n-Amyl n-butyrate
	n-Pentyl butanoate
	n-Pentyl butyrate
	n-Pentyl n-butyrate
Inchi:	InChI=1S/C9H18O2/c1-3-5-6-8-11-9(10)7-4-2/h3-8H2,1-2H3
InchiKey:	CFNJLPHOBMVMNS-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCOC(=O)CCC
Mol. weight [g/mol]:	158.24
CAS:	540-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-473.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1055.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1044.00		NIST Webbook

rinpol	1052.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1054.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1304.00		NIST Webbook
tb	451.75 ± 1.00	K	NIST Webbook

tb	449.00 ± 2.00	K	NIST Webbook
tb	459.50 ± 0.50	K	NIST Webbook
tc	655.29	K	Joback Method
tf	263.35	K	Joback Method
tt	200.48 ± 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	53.60	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56224e+01
Coeff. B	-4.21714e+03
Coeff. C	-6.85160e+01

Temperature range (K), min.	343.52
Temperature range (K), max.	477.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.34814e+01
Coeff. B	-6.74039e+03
Coeff. C	-3.98394e+00
Coeff. D	1.98902e-06
Temperature range (K), min.	365.15
Temperature range (K), max.	477.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1114.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540181&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1114
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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