1-METHYLBUTYL BUTYRATE

Other names:	1-methylbutyl butanoate
	2-Pentyl butanoate
	2-pentyl butyrate
	Butanoic acid, 2-pentyl ester
	Butyric acid, sec-pentyl ester
	UN 2620
	butanoic acid, 1-methylbutyl ester
	isopentyl butyrate
	sec-Amyl butyrate
Inchi:	InChI=1S/C9H18O2/c1-4-6-8(3)11-9(10)7-5-2/h8H,4-7H2,1-3H3
InchiKey:	DJOCFLQKCMWABC-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCC(=O)OC(C)CCC
Mol. weight [g/mol]:	158.24
CAS:	60415-61-4

Physical Properties

Property code	Value	Unit	Source
af	0.5356		Cheméo Relay (1.0)
hf	-570.58	kJ/mol	Cheméo Relay (1.0)
hfus	18.33	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1009.00		NIST Webbook

rinpol	1012.00		NIST Webbook
rinpol	999.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1214.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1214.00		NIST Webbook
tb	423.22	K	Cheméo Relay (1.0)
tc	614.52	K	Cheméo Relay (1.0)
tf	177.10	K	Cheméo Relay (1.0)
vc	0.551	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
rfi	1.40283		303.15	Liquid-liquid equilibria for ternary mixtures of 1-alkyl-3-methyl imidazolium bis{(trifluoromethyl)sulfonyl}imides, n-hexane and organic compounds at 303.15 K and 0.1 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42767e+01
Coeff. B	-3.77403e+03
Coeff. C	-6.57360e+01
Temperature range (K), min.	335.52
Temperature range (K), max.	486.70

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Liquid-liquid equilibria for ternary mixtures of 1-alkyl-3-methyl imidazolium bis{(trifluoromethyl)sulfonyl}imides, n-hexane and organic compounds at 303.15 K and 0.1 MPa:	https://www.doi.org/10.1016/j.jct.2016.08.033
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60415614&Units=SI
Cheméo Relay (1.0, beta):	
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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