

Butyl 2-methylbutanoate

Other names:	Butyl 2-methylbutyrate butanoic acid, 2-methyl-, butyl ester n-Butyl 2-methyl butyrate
Inchi:	InChI=1S/C9H18O2/c1-4-6-7-11-9(10)8(3)5-2/h8H,4-7H2,1-3H3
InchiKey:	OTKQNSSMCDLVQV-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCOC(=O)C(C)CC
Mol. weight [g/mol]:	158.24
CAS:	15706-73-7

Physical Properties

Property code	Value	Unit	Source
chl	-5504.50 ± 1.20	kJ/mol	NIST Webbook
gf	-211.46	kJ/mol	Joback Method
hf	-558.90 ± 1.30	kJ/mol	NIST Webbook
hfl	-609.50 ± 1.20	kJ/mol	NIST Webbook
hfus	18.33	kJ/mol	Joback Method
hvap	50.60 ± 0.50	kJ/mol	NIST Webbook
hvap	50.60	kJ/mol	NIST Webbook
hvap	50.57 ± 0.51	kJ/mol	NIST Webbook
hvap	54.40 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1042.00		NIST Webbook

rinpol	1038.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1030.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1219.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1232.00		NIST Webbook
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ripol	1241.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1240.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method

tf	248.35	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
dvisc	0.0020429	Paxs	287.15	Joback Method
dvisc	0.0010682	Paxs	325.96	Joback Method
dvisc	0.0006412	Paxs	364.76	Joback Method
dvisc	0.0004246	Paxs	403.56	Joback Method
dvisc	0.0003022	Paxs	442.37	Joback Method
dvisc	0.0047844	Paxs	248.35	Joback Method
dvisc	0.0002272	Paxs	481.17	Joback Method
pvap	0.67	kPa	319.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.55	kPa	316.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.43	kPa	313.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.31	kPa	308.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.21	kPa	303.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.15	kPa	298.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.10	kPa	293.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.07	kPa	288.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.05	kPa	283.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.04	kPa	280.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.03	kPa	278.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.03	kPa	276.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.02	kPa	274.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

Sources

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=C15706737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters:	https://www.doi.org/10.1016/j.fluid.2008.02.001

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
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

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