

Propanoic acid, 2,2-dimethyl-, butyl ester

Other names:	2,2-Dimethylpropionic acid, buthyl ester butyl 2,2-dimethylpropanoate butyl pivalate n-Butyl pivalate pivalic acid, butyl ester
Inchi:	InChI=1S/C9H18O2/c1-5-6-7-11-8(10)9(2,3)4/h5-7H2,1-4H3
InchiKey:	FCDMDSDBVPGGE-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCOC(=O)C(C)(C)C
Mol. weight [g/mol]:	158.24
CAS:	5129-37-3

Physical Properties

Property code	Value	Unit	Source
chl	-5497.70 ± 1.00	kJ/mol	NIST Webbook
gf	-206.18	kJ/mol	Joback Method
hf	-566.00 ± 1.10	kJ/mol	NIST Webbook
hfl	-616.40 ± 1.00	kJ/mol	NIST Webbook
hfus	14.44	kJ/mol	Joback Method
hvac	50.40 ± 0.30	kJ/mol	NIST Webbook
hvac	5552.00	kJ/mol	NIST Webbook
hvac	49.50 ± 0.20	kJ/mol	NIST Webbook
hvac	50.39 ± 0.34	kJ/mol	NIST Webbook
hvac	50.40	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mccol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
ripol	963.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1133.00		NIST Webbook
ripol	1133.00		NIST Webbook
tb	478.38	K	Joback Method
tc	662.57	K	Joback Method
tf	265.77	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.36	J/molxK	662.57	Joback Method
cpg	340.03	J/molxK	509.08	Joback Method
cpg	353.74	J/molxK	539.78	Joback Method
cpg	366.81	J/molxK	570.48	Joback Method
cpg	379.26	J/molxK	601.18	Joback Method
cpg	391.10	J/molxK	631.87	Joback Method
cpg	325.67	J/molxK	478.38	Joback Method
dvisc	0.0003187	Paxs	442.94	Joback Method
dvisc	0.0004508	Paxs	407.51	Joback Method
dvisc	0.0006812	Paxs	372.07	Joback Method
dvisc	0.0011229	Paxs	336.64	Joback Method
dvisc	0.0020820	Paxs	301.20	Joback Method
dvisc	0.0002372	Paxs	478.38	Joback Method
dvisc	0.0045510	Paxs	265.77	Joback Method
pvap	0.12	kPa	285.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.14	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.15	kPa	288.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.19	kPa	291.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.10	kPa	283.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.23	kPa	294.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.29	kPa	297.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.28	kPa	298.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.35	kPa	300.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.41	kPa	303.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.43	kPa	303.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.52	kPa	307.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.56	kPa	308.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.60	kPa	309.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.75	kPa	313.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.09	kPa	282.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.07	kPa	278.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.06	kPa	276.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.05	kPa	274.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.05	kPa	273.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.05	kPa	273.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap

0.21

kPa

293.20

Transpiration
method: Vapor
pressures and
enthalpies of
vaporization of
some low-boiling
esters

Sources

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
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=C5129373&Units=SI

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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