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: FCDMDSDHBVPGGE-UHFFFAOYSA-N

Formula: C9H18O2

SMILES: CCCCOC(=O)C(C)(C)C

Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
af	0.4937		Cheméo Relay (1.0)
chl	-5497.70 ± 1.00	kJ/mol	NIST Webbook
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
hvap	49.50 ± 0.20	kJ/mol	NIST Webbook
hvap	50.39 ± 0.34	kJ/mol	NIST Webbook
hvap	50.40	kJ/mol	NIST Webbook
hvap	50.40 ± 0.30	kJ/mol	NIST Webbook
hvap	5552.00	kJ/mol	NIST Webbook
ie	9.71	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	965.00		NIST Webbook
ripol	1133.00		NIST Webbook
ripol	1128.00		NIST Webbook
ripol	1133.00		NIST Webbook
tb	428.30	K	Cheméo Relay (1.0)
tc	605.07	K	Cheméo Relay (1.0)
tf	190.55	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	402.36	J/mol×K	662.57	Joback Method
cpg	340.03	J/mol×K	509.08	Joback Method
cpg	353.74	J/mol×K	539.78	Joback Method
cpg	325.67	J/mol×K	478.38	Joback Method
cpg	366.81	J/mol×K	570.48	Joback Method
cpg	379.26	J/mol×K	601.18	Joback Method
cpg	391.10	J/mol×K	631.87	Joback Method
dvisc	0.0004508	Pa×s	407.51	Joback Method
dvisc	0.0045510	Pa×s	265.77	Joback Method
dvisc	0.0020820	Pa×s	301.20	Joback Method
dvisc	0.0011229	Pa×s	336.64	Joback Method
dvisc	0.0006812	Pa×s	372.07	Joback Method
dvisc	0.0003187	Pa×s	442.94	Joback Method
dvisc	0.0002372	Pa×s	478.38	Joback Method
pvap	0.15	kPa	288.70	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
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	0.28	kPa	298.10	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	0.23	kPa	294.80	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	0.19	kPa	291.70	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	0.14	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.12	kPa	285.60	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	0.09	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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters:	https://www.doi.org/10.1016/j.fluid.2008.02.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129373&Units=SI
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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
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