Butyric acid, neopentyl ester

Other names:	1,1-dimethylpropyl butanoate
	UN 2620
	butanoic acid, 1,1-dimethylpropyl ester
	tert-Amyl butyrate
	tert-pentyl butyrate
Inchi:	InChI=1S/C9H18O2/c1-5-7-8(10)11-9(3,4)6-2/h5-7H2,1-4H3
InchiKey:	VTZSXMMBJHMLEE-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCC(=O)OC(C)(C)CC
Mol. weight [g/mol]:	158.24
CAS:	2050-00-2

Physical Properties

Property code	Value	Unit	Source
chl	-5489.28 ± 0.98	kJ/mol	NIST Webbook
gf	-206.18	kJ/mol	Joback Method
hf	-574.00 ± 1.10	kJ/mol	NIST Webbook
hfl	-624.80 ± 1.00	kJ/mol	NIST Webbook
hfus	14.44	kJ/mol	Joback Method
hvap	48.90	kJ/mol	NIST Webbook
hvap	50.84 ± 0.57	kJ/mol	NIST Webbook
hvap	50.80	kJ/mol	NIST Webbook
hvap	50.80 ± 0.60	kJ/mol	NIST Webbook
hvap	50.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	972.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1178.00		NIST Webbook
tb	478.38	K	Joback Method

tc	662.57	K	Joback Method
tf	265.77	K	Joback Method
vc	0.552	m3/kmol	Joback Method

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	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
cpg	325.67	J/mol×K	478.38	Joback Method
dvisc	0.0003187	Pa×s	442.94	Joback Method
dvisc	0.0004508	Pa×s	407.51	Joback Method
dvisc	0.0006812	Pa×s	372.07	Joback Method
dvisc	0.0011229	Pa×s	336.64	Joback Method
dvisc	0.0020820	Pa×s	301.20	Joback Method
dvisc	0.0002372	Pa×s	478.38	Joback Method
dvisc	0.0045510	Pa×s	265.77	Joback Method
pvap	0.11	kPa	285.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.15	kPa	288.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.14	kPa	288.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.10	kPa	283.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.20	kPa	293.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.22	kPa	294.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.27	kPa	297.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.29	kPa	298.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.33	kPa	300.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.41	kPa	303.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.40	kPa	303.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.49	kPa	306.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.56	kPa	308.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.59	kPa	309.50	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	0.08	kPa	280.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.07	kPa	278.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.07	kPa	278.20	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	274.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.18	kPa	291.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2050002&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