

Butanoic acid, 3,3-dimethyl-, methyl ester

Other names:	Methyl 3,3-dimethylbutyrate butyric acid, 3,3-dimethyl-, methyl ester methyl 3,3-dimethylbutanoate methyl tert-butylacetate
Inchi:	InChI=1S/C7H14O2/c1-7(2,3)5-6(8)9-4/h5H2,1-4H3
InchiKey:	DXBOTVWRXLQVMG-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	COC(=O)CC(C)(C)C
Mol. weight [g/mol]:	130.18
CAS:	10250-48-3

Physical Properties

Property code	Value	Unit	Source
chl	-4199.20 ± 1.60	kJ/mol	NIST Webbook
gf	-223.02	kJ/mol	Joback Method
hf	-511.70 ± 1.60	kJ/mol	NIST Webbook
hfl	-556.10 ± 1.60	kJ/mol	NIST Webbook
hfus	9.26	kJ/mol	Joback Method
hvap	44.39 ± 0.16	kJ/mol	NIST Webbook
hvac	43.90 ± 0.20	kJ/mol	NIST Webbook
hvac	44.40	kJ/mol	NIST Webbook
hvac	44.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mccol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	400.00 ± 1.00	K	NIST Webbook
tc	620.42	K	Joback Method
tf	243.23	K	Joback Method
vc	0.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	241.05	J/molxK	432.62	Joback Method
cpg	253.38	J/molxK	463.92	Joback Method
cpg	265.15	J/molxK	495.22	Joback Method
cpg	276.37	J/molxK	526.52	Joback Method
cpg	287.06	J/molxK	557.82	Joback Method
cpg	297.22	J/molxK	589.12	Joback Method
cpg	306.89	J/molxK	620.42	Joback Method
dvisc	0.0047587	Paxs	243.23	Joback Method
dvisc	0.0022582	Paxs	274.80	Joback Method
dvisc	0.0012495	Paxs	306.36	Joback Method
dvisc	0.0007722	Paxs	337.93	Joback Method
dvisc	0.0005181	Paxs	369.49	Joback Method
dvisc	0.0003702	Paxs	401.06	Joback Method
dvisc	0.0002778	Paxs	432.62	Joback Method
pvap	0.46	kPa	279.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.32	kPa	274.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.35	kPa	275.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.40	kPa	277.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.44	kPa	278.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.30	kPa	273.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.52	kPa	281.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.57	kPa	282.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.59	kPa	283.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.69	kPa	285.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.82	kPa	288.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.82	kPa	288.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.00	kPa	291.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.13	kPa	293.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.19	kPa	294.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	1.44	kPa	297.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.53	kPa	298.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.85	kPa	301.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.04	kPa	303.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.09	kPa	303.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.50	kPa	306.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.74	kPa	308.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.78	kPa	309.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap

3.59

kPa

313.20

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

Sources

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=C10250483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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