

Butanoic acid, 3-methyl, 1,1-dimethylethyl ester

Other names:	isovaleric acid, tert-butyl ester
Inchi:	InChI=1S/C9H18O2/c1-7(2)6-8(10)11-9(3,4)5/h7H,6H2,1-5H3
InchiKey:	ZKAODOPIAGAVNQ-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CC(C)CC(=O)OC(C)(C)C
Mol. weight [g/mol]:	158.24
CAS:	16792-03-3

Physical Properties

Property code	Value	Unit	Source
gf	-208.62	kJ/mol	Joback Method
hf	-487.92	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	912.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1073.00		NIST Webbook
tb	477.94	K	Joback Method
tc	666.16	K	Joback Method
tf	250.77	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.82	J/molxK	477.94	Joback Method
cpg	392.85	J/molxK	634.79	Joback Method
cpg	380.76	J/molxK	603.42	Joback Method
cpg	368.03	J/molxK	572.05	Joback Method
cpg	354.64	J/molxK	540.68	Joback Method

cpg	340.58	J/mol×K	509.31	Joback Method
cpg	404.33	J/mol×K	666.16	Joback Method
dvisc	0.0002253	Paxs	477.94	Joback Method
dvisc	0.0003117	Paxs	440.08	Joback Method
dvisc	0.0004585	Paxs	402.22	Joback Method
dvisc	0.0007309	Paxs	364.36	Joback Method
dvisc	0.0012980	Paxs	326.49	Joback Method
dvisc	0.0026801	Paxs	288.63	Joback Method
dvisc	0.0068881	Paxs	250.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16792033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
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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