

Butanoic acid, 2,2,3,3-tetramethyl, ethyl ester

Inchi:	InChI=1S/C10H20O2/c1-7-12-8(11)10(5,6)9(2,3)4/h7H2,1-6H3
InchiKey:	ISDTWPKODWTCFS-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCOC(=O)C(C)(C)C(C)(C)C
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-194.92	kJ/mol	Joback Method
hf	-512.03	kJ/mol	Joback Method
hfus	9.62	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	987.00		NIST Webbook
tb	498.03	K	Joback Method
tc	691.51	K	Joback Method
tf	279.46	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.79	J/molxK	498.03	Joback Method
cpg	390.18	J/molxK	530.28	Joback Method
cpg	405.67	J/molxK	562.52	Joback Method
cpg	420.29	J/molxK	594.77	Joback Method
cpg	434.08	J/molxK	627.01	Joback Method
cpg	447.08	J/molxK	659.26	Joback Method
cpg	459.32	J/molxK	691.51	Joback Method
dvisc	0.0056934	Paxs	279.46	Joback Method
dvisc	0.0023921	Paxs	315.89	Joback Method

dvisc	0.0012024	Paxs	352.32	Joback Method
dvisc	0.0006876	Paxs	388.75	Joback Method
dvisc	0.0004327	Paxs	425.17	Joback Method
dvisc	0.0002929	Paxs	461.60	Joback Method
dvisc	0.0002100	Paxs	498.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108155&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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