

# Propionic acid, 3,3-diethoxy-2,2-dimethyl-, ethyl ester

Inchi:	InChI=1S/C11H22O4/c1-6-13-9(12)11(4,5)10(14-7-2)15-8-3/h10H,6-8H2,1-5H3
InchiKey:	NCXYMZLOQQCRW-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CCOC(=O)C(C)(C)C(OCC)OCC
Mol. weight [g/mol]:	218.29
CAS:	116594-66-2

## Physical Properties

Property code	Value	Unit	Source
gf	-401.78	kJ/mol	Joback Method
hf	-793.64	kJ/mol	Joback Method
hfus	18.47	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.975		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
tb	568.54	K	Joback Method
tc	750.68	K	Joback Method
tf	317.77	K	Joback Method
vc	0.695	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.73	J/molxK	568.54	Joback Method
cpg	544.41	J/molxK	720.32	Joback Method
cpg	531.41	J/molxK	689.97	Joback Method
cpg	517.74	J/molxK	659.61	Joback Method
cpg	503.41	J/molxK	629.25	Joback Method
cpg	488.41	J/molxK	598.90	Joback Method
cpg	556.74	J/molxK	750.68	Joback Method
dvisc	0.0001131	Paxs	568.54	Joback Method
dvisc	0.0001545	Paxs	526.74	Joback Method

dvisc	0.0002228	Paxs	484.95	Joback Method
dvisc	0.0003442	Paxs	443.15	Joback Method
dvisc	0.0005823	Paxs	401.36	Joback Method
dvisc	0.0011130	Paxs	359.56	Joback Method
dvisc	0.0025227	Paxs	317.77	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116594662&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116594662&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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