

# Propanoic acid, 2-iodoethyl ester

Inchi:	InChI=1S/C5H9IO2/c1-2-5(7)8-4-3-6/h2-4H2,1H3
InchiKey:	YXIMMRXXZQYICY-UHFFFAOYSA-N
Formula:	C5H9IO2
SMILES:	CCC(=O)OCCI
Mol. weight [g/mol]:	228.03

## Physical Properties

Property code	Value	Unit	Source
gf	-184.58	kJ/mol	Joback Method
hf	-314.46	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	45.25	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.375		Crippen Method
mcvol	114.570	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpola	1063.00		NIST Webbook
tb	483.23	K	Joback Method
tc	696.06	K	Joback Method
tf	276.33	K	Joback Method
vc	0.427	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.12	J/molxK	483.23	Joback Method
cpg	244.50	J/molxK	660.59	Joback Method
cpg	237.42	J/molxK	625.12	Joback Method
cpg	229.94	J/molxK	589.64	Joback Method
cpg	222.07	J/molxK	554.17	Joback Method
cpg	213.80	J/molxK	518.70	Joback Method
cpg	251.21	J/molxK	696.06	Joback Method
dvisc	0.0003583	Paxs	483.23	Joback Method
dvisc	0.0004552	Paxs	448.75	Joback Method

dvisc	0.0006017	Paxs	414.26	Joback Method
dvisc	0.0008369	Paxs	379.78	Joback Method
dvisc	0.0012431	Paxs	345.30	Joback Method
dvisc	0.0020161	Paxs	310.81	Joback Method
dvisc	0.0036892	Paxs	276.33	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R20053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R20053&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>rinpol:</b>	Non-polar retention indices
<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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