

# Propionic acid, 3-iodo-, octyl ester

<b>Inchi:</b>	InChI=1S/C11H21IO2/c1-2-3-4-5-6-7-10-14-11(13)8-9-12/h2-10H2,1H3
<b>InchiKey:</b>	IBTOBYKVXQPQGO-UHFFFAOYSA-N
<b>Formula:</b>	C11H21IO2
<b>SMILES:</b>	CCCCCCCCOC(=O)CCI
<b>Mol. weight [g/mol]:</b>	312.19

## Physical Properties

Property code	Value	Unit	Source
gf	-134.06	kJ/mol	Joback Method
hf	-438.30	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.715		Crippen Method
mvol	199.110	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	620.51	K	Joback Method
tc	815.62	K	Joback Method
tf	343.95	K	Joback Method
vc	0.763	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.09	J/molxK	620.51	Joback Method
cpg	541.13	J/molxK	783.11	Joback Method
cpg	529.48	J/molxK	750.59	Joback Method
cpg	517.16	J/molxK	718.07	Joback Method
cpg	504.17	J/molxK	685.55	Joback Method
cpg	490.49	J/molxK	653.03	Joback Method
cpg	552.15	J/molxK	815.62	Joback Method
dvisc	0.0001855	Paxs	620.51	Joback Method

dvisc	0.0002424	Paxs	574.42	Joback Method
dvisc	0.0003320	Paxs	528.32	Joback Method
dvisc	0.0004827	Paxs	482.23	Joback Method
dvisc	0.0007598	Paxs	436.14	Joback Method
dvisc	0.0013314	Paxs	390.04	Joback Method
dvisc	0.0027112	Paxs	343.95	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=U406243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406243&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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