

# 3-Iodopentane

Inchi:	InChI=1S/C5H11I/c1-3-5(6)4-2/h5H,3-4H2,1-2H3
InchiKey:	VRQDQJYBWZERBW-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CCC(I)CC
Mol. weight [g/mol]:	198.05
CAS:	1809-05-8

## Physical Properties

Property code	Value	Unit	Source
gf	46.90	kJ/mol	Joback Method
hf	-74.94	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.610		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpola	876.00		NIST Webbook
ripola	1093.00		NIST Webbook
ripola	1093.00		NIST Webbook
tb	406.50	K	Joback Method
tc	613.94	K	Joback Method
tf	189.17	K	Joback Method
vc	0.398	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.15	J/molxK	406.50	Joback Method
cpg	182.14	J/molxK	441.07	Joback Method
cpg	191.61	J/molxK	475.65	Joback Method
cpg	200.59	J/molxK	510.22	Joback Method
cpg	209.09	J/molxK	544.79	Joback Method
cpg	217.13	J/molxK	579.36	Joback Method

cpg	224.75	J/molxK	613.94	Joback Method
dvisc	0.0102765	Paxs	189.17	Joback Method
dvisc	0.0037890	Paxs	225.39	Joback Method
dvisc	0.0018416	Paxs	261.61	Joback Method
dvisc	0.0010668	Paxs	297.84	Joback Method
dvisc	0.0006956	Paxs	334.06	Joback Method
dvisc	0.0004932	Paxs	370.28	Joback Method
dvisc	0.0003718	Paxs	406.50	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	6.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38831e+01
Coeff. B	-3.42776e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	309.52
Temperature range (K), max.	457.29

## 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=C1809058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809058&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

# 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>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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