

# Docosane, 1-iodo-

<b>Inchi:</b>	InChI=1S/C22H45I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h2-2
<b>InchiKey:</b>	QQTWESGWRGHHPL-UHFFFAOYSA-N
<b>Formula:</b>	C22H45I
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	436.50

## Physical Properties

Property code	Value	Unit	Source
gf	192.48	kJ/mol	Joback Method
hf	-420.54	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	73.94	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.243		Crippen Method
mcvol	346.660	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinsol	2730.00		NIST Webbook
tb	795.90	K	Joback Method
tc	979.42	K	Joback Method
tf	395.76	K	Joback Method
vc	1.355	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.95	J/molxK	795.90	Joback Method
cpg	1064.48	J/molxK	826.49	Joback Method
cpg	1084.01	J/molxK	857.07	Joback Method
cpg	1102.59	J/molxK	887.66	Joback Method
cpg	1120.27	J/molxK	918.25	Joback Method
cpg	1137.11	J/molxK	948.84	Joback Method
cpg	1153.14	J/molxK	979.42	Joback Method
dvisc	0.0017848	Paxs	395.76	Joback Method
dvisc	0.0006583	Paxs	462.45	Joback Method

dvisc	0.0003122	Paxs	529.14	Joback Method
dvisc	0.0001750	Paxs	595.83	Joback Method
dvisc	0.0001102	Paxs	662.52	Joback Method
dvisc	0.0000755	Paxs	729.21	Joback Method
dvisc	0.0000551	Paxs	795.90	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406319&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406319&amp;Units=SI</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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