

Nonane, 1-iodo-

Other names:	1-Iodononane 1-n-Nonyl iodide Nonyl iodide n-Nonyl iodide
Inchi:	InChI=1S/C9H19I/c1-2-3-4-5-6-7-8-9-10/h2-9H2,1H3
InchiKey:	OGSJMFCWOUHXHN-UHFFFAOYSA-N
Formula:	C9H19I
SMILES:	CCCCCCCCCI
Mol. weight [g/mol]:	254.15
CAS:	4282-42-2

Physical Properties

Property code	Value	Unit	Source
gf	83.02	kJ/mol	Joback Method
hf	-152.22	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	64.50	kJ/mol	NIST Webbook
log10ws	-4.54		Crippen Method
logp	4.172		Crippen Method
mcvol	163.490	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
ripol	1327.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1600.00		NIST Webbook
tb	498.46	K	Joback Method
tc	691.87	K	Joback Method
tf	249.25	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	334.79	J/molxK	498.46	Joback Method
cpg	349.05	J/molxK	530.69	Joback Method
cpg	362.63	J/molxK	562.93	Joback Method
cpg	375.55	J/molxK	595.16	Joback Method
cpg	387.83	J/molxK	627.40	Joback Method
cpg	399.51	J/molxK	659.63	Joback Method
cpg	410.61	J/molxK	691.87	Joback Method
dvisc	0.0024915	Paxs	290.79	Joback Method
dvisc	0.0059305	Paxs	249.25	Joback Method
dvisc	0.0013001	Paxs	332.32	Joback Method
dvisc	0.0007839	Paxs	373.86	Joback Method
dvisc	0.0005230	Paxs	415.39	Joback Method
dvisc	0.0003755	Paxs	456.93	Joback Method
dvisc	0.0002850	Paxs	498.46	Joback Method
hvapt	54.60	kJ/mol	471.00	NIST Webbook
hvapt	53.50	kJ/mol	492.50	NIST Webbook
hvapt	64.30	kJ/mol	418.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61999e+01
Coeff. B	-4.84249e+03
Coeff. C	-8.51960e+01
Temperature range (K), min.	389.52
Temperature range (K), max.	529.93

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4282422&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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