

Decane, 1-iodo-

Other names:	1-Decyl iodide 1-Iododecane 1-Iododecane Decyl iodide n-Decyl iodide
Inchi:	InChI=1S/C10H21I/c1-2-3-4-5-6-7-8-9-10-11/h2-10H2,1H3
InchiKey:	SKIDNYUZJPMKFC-UHFFFAOYSA-N
Formula:	C10H21I
SMILES:	CCCCCCCCCI
Mol. weight [g/mol]:	268.18
CAS:	2050-77-3

Physical Properties

Property code	Value	Unit	Source
gf	91.44	kJ/mol	Joback Method
hf	-172.86	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	69.80	kJ/mol	NIST Webbook
log10ws	-4.96		Crippen Method
logp	4.562		Crippen Method
mcvol	177.580	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1433.00		NIST Webbook
rinpol	1433.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1734.00		NIST Webbook
tb	521.34	K	Joback Method
tc	712.37	K	Joback Method
tf	260.52	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.50	J/molxK	521.34	Joback Method
cpg	395.60	J/molxK	553.18	Joback Method
cpg	409.98	J/molxK	585.02	Joback Method
cpg	423.67	J/molxK	616.86	Joback Method
cpg	436.69	J/molxK	648.70	Joback Method
cpg	449.07	J/molxK	680.54	Joback Method
cpg	460.85	J/molxK	712.37	Joback Method
dvisc	0.0023427	Paxs	303.99	Joback Method
dvisc	0.0056611	Paxs	260.52	Joback Method
dvisc	0.0012089	Paxs	347.46	Joback Method
dvisc	0.0007228	Paxs	390.93	Joback Method
dvisc	0.0004789	Paxs	434.40	Joback Method
dvisc	0.0003421	Paxs	477.87	Joback Method
dvisc	0.0002584	Paxs	521.34	Joback Method
hvapt	57.40	kJ/mol	489.00	NIST Webbook
hvapt	58.10	kJ/mol	497.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37437e+01
Coeff. B	-4.22636e+03
Coeff. C	-9.03940e+01
Temperature range (K), min.	404.48
Temperature range (K), max.	591.61

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050773&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/ci990307I
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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