1-Iodoundecane

Other names: Undecane, 1-iodo-
Inchi: InChI=1S/C11H23I/c1-2-3-4-5-6-7-8-9-10-11-12/h2-11H2,1H3
InchiKey: FKUQOQPBCHJHAP-UHFFFAOYSA-N
Formula: C11H23I
SMILES: CCCCCCCCCCCI
Mol. weight [g/mol]: 282.20
CAS: 4282-44-4

Physical Properties

Property code	Value	Unit	Source
gf	99.86	kJ/mol	Joback Method
hf	-193.50	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	74.80	kJ/mol	NIST Webbook
log10ws	-5.38		Crippen Method
logp	4.952		Crippen Method
mcvol	191.670	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1537.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1816.00		NIST Webbook
tb	544.22	K	Joback Method
tc	732.96	K	Joback Method
tf	271.79	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.96	J/mol×K	701.50	Joback Method
cpg	512.33	J/mol×K	732.96	Joback Method

cpg	428.03	J/mol×K	544.22	Joback Method
cpg	443.86	J/mol×K	575.68	Joback Method
cpg	458.94	J/mol×K	607.13	Joback Method
cpg	473.30	J/mol×K	638.59	Joback Method
cpg	486.96	J/mol×K	670.05	Joback Method
dvisc	0.0002327	Pa×s	544.22	Joback Method
dvisc	0.0003094	Pa×s	498.81	Joback Method
dvisc	0.0053452	Pa×s	271.79	Joback Method
dvisc	0.0021814	Pa×s	317.19	Joback Method
dvisc	0.0011143	Pa×s	362.60	Joback Method
dvisc	0.0006610	Pa×s	408.00	Joback Method
dvisc	0.0004353	Pa×s	453.41	Joback Method
hvapt	60.90	kJ/mol	515.00	NIST Webbook
hvapt	60.10	kJ/mol	505.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64657e+01
Coeff. B	-5.23165e+03
Coeff. C	-9.53430e+01
Temperature range (K), min.	418.72
Temperature range (K), max.	564.37

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4282444&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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