Octadecane, 1-iodo-

Other names:	1-Iodooctadecane
	Octadecyl iodide
	Stearyl iodide
	n-Octadecyl iodide
Inchi:	InChI=1S/C18H37I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-18H2,1H3
InchiKey:	ZNJOCVLVYVOUGB-UHFFFAOYSA-N
Formula:	C18H37I
SMILES:	CCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]:	380.39
CAS:	629-93-6

Physical Properties

Property code	Value	Unit	Source
gf	158.80	kJ/mol	Joback Method
hf	-337.98	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	109.30	kJ/mol	NIST Webbook
log10ws	-8.31		Crippen Method
logp	7.683		Crippen Method
mcvol	290.300	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2290.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2272.00		NIST Webbook
ripol	2576.00		NIST Webbook
tb	656.20	K	NIST Webbook
tc	883.65	K	Joback Method
tf	307.00 ± 3.00	K	NIST Webbook
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	905.12	J/mol×K	883.65	Joback Method
cpg	890.14	J/mol×K	853.77	Joback Method
cpg	874.42	J/mol×K	823.90	Joback Method
cpg	857.92	J/mol×K	794.02	Joback Method
cpg	840.60	J/mol×K	764.14	Joback Method
cpg	822.42	J/mol×K	734.26	Joback Method
cpg	803.35	J/mol×K	704.38	Joback Method
dvisc	0.0028659	Pa×s	350.68	Joback Method
dvisc	0.0000975	Pa×s	704.38	Joback Method
dvisc	0.0001325	Pa×s	645.43	Joback Method
dvisc	0.0001913	Pa×s	586.48	Joback Method
dvisc	0.0003000	Pa×s	527.53	Joback Method
dvisc	0.0005268	Pa×s	468.58	Joback Method
dvisc	0.0010877	Pa×s	409.63	Joback Method
hvapt	77.20	kJ/mol	584.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	468.70	K	0.30	NIST Webbook
tbrp	468.50 ± 1.50	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63563e+01
Coeff. B	-6.04763e+03
Coeff. C	-1.23560e+02
Temperature range (K), min.	499.92
Temperature range (K), max.	671.11

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629936&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
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