Octane, 1-iodo-

Other names:	1-Iodooctane
	1-Jodoktan
	1-Octyl iodide
	1-n-Octyl iodide
	Octyl iodide
	n-Octyl iodide
Inchi:	InChI=1S/C8H17I/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3
InchiKey:	UWLHSHAHTBJTBA-UHFFFAOYSA-N
Formula:	C8H17I
SMILES:	CCCCCCCCI
Mol. weight [g/mol]:	240.12
CAS:	629-27-6

Physical Properties

Property code	Value	Unit	Source
gf	74.60	kJ/mol	Joback Method
hf	-131.58	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	59.70	kJ/mol	NIST Webbook
log10ws	-4.12		Crippen Method
logp	3.782		Crippen Method
mcvol	149.400	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1225.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	498.70	K	NIST Webbook
tb	499.15 ± 0.60	K	NIST Webbook
tc	671.37	K	Joback Method
tf	227.45 ± 0.50	K	NIST Webbook
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.67	J/mol×K	671.37	Joback Method
cpg	290.98	J/mol×K	475.58	Joback Method
cpg	304.29	J/mol×K	508.21	Joback Method
cpg	316.96	J/mol×K	540.84	Joback Method
cpg	329.00	J/mol×K	573.48	Joback Method
cpg	340.45	J/mol×K	606.11	Joback Method
cpg	351.33	J/mol×K	638.74	Joback Method
dvisc	0.0003119	Pa×s	475.58	Joback Method
dvisc	0.0061362	Pa×s	237.98	Joback Method
dvisc	0.0026208	Pa×s	277.58	Joback Method
dvisc	0.0013843	Pa×s	317.18	Joback Method
dvisc	0.0008425	Pa×s	356.78	Joback Method
dvisc	0.0005662	Pa×s	396.38	Joback Method
dvisc	0.0004090	Pa×s	435.98	Joback Method
hvapt	50.70	kJ/mol	472.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.70	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47947e+01
Coeff. B	-4.26424e+03
Coeff. C	-7.96660e+01
Temperature range (K), min.	373.61
Temperature range (K), max.	529.33

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629276&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

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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