Octane, 2-iodo-

Other names:	2-Iodooctane
	2-Octyl iodide
	sec-Octyl Iodide
Inchi:	InChI=1S/C8H17I/c1-3-4-5-6-7-8(2)9/h8H,3-7H2,1-2H3
InchiKey:	XFLOGTUFKZCFTK-UHFFFAOYSA-N
Formula:	C8H17I
SMILES:	CCCCCCC(C)I
Mol. weight [g/mol]:	240.12
CAS:	557-36-8

Physical Properties

Property code	Value	Unit	Source
gf	72.16	kJ/mol	Joback Method
hf	-136.86	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.780		Crippen Method
mcvol	149.400	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1119.00		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	475.14	K	Joback Method
tc	675.39	K	Joback Method
tf	222.98	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.15	J/mol×K	475.14	Joback Method
cpg	353.06	J/mol×K	642.01	Joback Method
cpg	341.94	J/mol×K	608.64	Joback Method
cpg	330.22	J/mol×K	575.26	Joback Method

cpg	317.86	J/mol×K	541.89	Joback Method
cpg	304.85	J/mol×K	508.51	Joback Method
cpg	363.61	J/mol×K	675.39	Joback Method
dvisc	0.0002962	Pa×s	475.14	Joback Method
dvisc	0.0003989	Pa×s	433.11	Joback Method
dvisc	0.0005725	Pa×s	391.09	Joback Method
dvisc	0.0008966	Pa×s	349.06	Joback Method
dvisc	0.0015876	Pa×s	307.03	Joback Method
dvisc	0.0033695	Pa×s	265.01	Joback Method
dvisc	0.0094969	Pa×s	222.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46081e+01
Coeff. B	-4.09643e+03
Coeff. C	-7.54660e+01
Temperature range (K), min.	361.52
Temperature range (K), max.	516.10

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C557368&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume