Hexane, 3-iodo-

Other names: 3-Iodohexane
Inchi: InChI=1S/C6H13I/c1-3-5-6(7)4-2/h6H,3-5H2,1-2H3
InchiKey: QQKICFXKOIDMSQ-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CCCC(I)CC
Mol. weight [g/mol]: 212.07
CAS: 31294-91-4

Physical Properties

Property code	Value	Unit	Source
gf	55.32	kJ/mol	Joback Method
hf	-95.58	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	37.94	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.000		Crippen Method
mcvol	121.220	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	1036.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1182.00		NIST Webbook
tb	429.38	K	Joback Method
tc	634.59	K	Joback Method
tf	200.44	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.62	J/mol×K	429.38	Joback Method
cpg	260.91	J/mol×K	600.38	Joback Method

cpg	251.72	J/mol×K	566.18	Joback Method
cpg	242.02	J/mol×K	531.98	Joback Method
cpg	231.78	J/mol×K	497.78	Joback Method
cpg	220.99	J/mol×K	463.58	Joback Method
cpg	269.61	J/mol×K	634.59	Joback Method
dvisc	0.0003483	Pa×s	429.38	Joback Method
dvisc	0.0004646	Pa×s	391.22	Joback Method
dvisc	0.0006596	Pa×s	353.07	Joback Method
dvisc	0.0010195	Pa×s	314.91	Joback Method
dvisc	0.0017766	Pa×s	276.75	Joback Method
dvisc	0.0036980	Pa×s	238.60	Joback Method
dvisc	0.0101753	Pa×s	200.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41725e+01
Coeff. B	-3.66743e+03
Coeff. C	-6.37900e+01
Temperature range (K), min.	327.92
Temperature range (K), max.	477.67

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=C31294914&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume