Hexane, 2-iodo-

Other names: 2-Iodohexane
Inchi: InChI=1S/C6H13I/c1-3-4-5-6(2)7/h6H,3-5H2,1-2H3
InchiKey: XCEDNORUDUKWGK-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CCCCC(C)I
Mol. weight [g/mol]: 212.07
CAS: 18589-27-0

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	1037.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	1037.00		NIST Webbook
ripol	1186.00		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	1.42558e+01
Coeff. B	-3.69672e+03
Coeff. C	-6.40680e+01
Temperature range (K), min.	328.72
Temperature range (K), max.	477.37

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=C18589270&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