Heptane, 3-iodo-

Other names: 3-Iodoheptane
Inchi: InChI=1S/C7H15I/c1-3-5-6-7(8)4-2/h7H,3-6H2,1-2H3
InchiKey: LVPGHYVXKUXNQR-UHFFFAOYSA-N
Formula: C7H15I
SMILES: CCCCC(I)CC
Mol. weight [g/mol]: 226.10
CAS: 31294-92-5

Physical Properties

Property code	Value	Unit	Source
gf	63.74	kJ/mol	Joback Method
hf	-116.22	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.390		Crippen Method
mcvol	135.310	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1071.00		NIST Webbook
ripol	1270.00		NIST Webbook
tb	452.26	K	Joback Method
tc	655.04	K	Joback Method
tf	211.71	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.32	J/mol×K	452.26	Joback Method
cpg	306.24	J/mol×K	621.25	Joback Method
cpg	296.03	J/mol×K	587.45	Joback Method
cpg	285.26	J/mol×K	553.65	Joback Method
cpg	273.90	J/mol×K	519.85	Joback Method

cpg	261.93	J/mol×K	486.06	Joback Method
cpg	315.92	J/mol×K	655.04	Joback Method
dvisc	0.0003227	Pa×s	452.26	Joback Method
dvisc	0.0004326	Pa×s	412.17	Joback Method
dvisc	0.0006178	Pa×s	372.08	Joback Method
dvisc	0.0009615	Pa×s	331.99	Joback Method
dvisc	0.0016897	Pa×s	291.89	Joback Method
dvisc	0.0035535	Pa×s	251.80	Joback Method
dvisc	0.0099031	Pa×s	211.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47819e+01
Coeff. B	-4.02472e+03
Coeff. C	-7.10040e+01
Temperature range (K), min.	348.68
Temperature range (K), max.	495.98

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=C31294925&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume