

Heptane, 2-iodo-

Other names:	2-Iodoheptane
Inchi:	InChI=1S/C7H15I/c1-3-4-5-6-7(2)8/h7H,3-6H2,1-2H3
InchiKey:	QAUTWECDRZFXMN-UHFFFAOYSA-N
Formula:	C7H15I
SMILES:	CCCCC(C)I
Mol. weight [g/mol]:	226.10
CAS:	18589-29-2

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	1136.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1280.00		NIST Webbook
tb	452.26	K	Joback Method
tc	655.04	K	Joback Method
tf	211.71	K	Joback Method
vc	0.509	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.32	J/molxK	452.26	Joback Method
cpg	306.24	J/molxK	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	Paxs	452.26	Joback Method
dvisc	0.0004326	Paxs	412.17	Joback Method
dvisc	0.0006178	Paxs	372.08	Joback Method
dvisc	0.0009615	Paxs	331.99	Joback Method
dvisc	0.0016897	Paxs	291.89	Joback Method
dvisc	0.0035535	Paxs	251.80	Joback Method
dvisc	0.0099031	Paxs	211.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C18589292&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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