Pentane, 2-iodo-2-methyl

Other names: 2-Iodo-2-methylpentane
Inchi: InChI=1S/C6H13I/c1-4-5-6(2,3)7/h4-5H2,1-3H3
InchiKey: KCNIMEJTKUGMLA-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CCCC(C)(C)I
Mol. weight [g/mol]: 212.07
CAS: 31294-95-8

Physical Properties

Property code	Value	Unit	Source
gf	60.60	kJ/mol	Joback Method
hf	-99.05	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	37.03	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.000		Crippen Method
mcvol	121.220	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1171.00		NIST Webbook
tb	426.59	K	Joback Method
tc	640.95	K	Joback Method
tf	217.86	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.97	J/mol×K	426.59	Joback Method
cpg	224.35	J/mol×K	462.32	Joback Method
cpg	235.92	J/mol×K	498.04	Joback Method
cpg	246.73	J/mol×K	533.77	Joback Method

cpg	256.82	J/mol×K	569.49	Joback Method
cpg	266.25	J/mol×K	605.22	Joback Method
cpg	275.05	J/mol×K	640.95	Joback Method
dvisc	0.0104269	Pa×s	217.86	Joback Method
dvisc	0.0041142	Pa×s	252.65	Joback Method
dvisc	0.0020332	Pa×s	287.44	Joback Method
dvisc	0.0011699	Pa×s	322.23	Joback Method
dvisc	0.0007498	Pa×s	357.01	Joback Method
dvisc	0.0005200	Pa×s	391.80	Joback Method
dvisc	0.0003828	Pa×s	426.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46093e+01
Coeff. B	-3.82093e+03
Coeff. C	-6.52070e+01
Temperature range (K), min.	332.00
Temperature range (K), max.	476.16

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=R25558&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