Pentane, 3-iodo-2-methyl

Inchi: InChI=1S/C6H13I/c1-4-6(7)5(2)3/h5-6H,4H2,1-3H3
InchiKey: AEKOVZFTJZYZRS-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CCC(I)C(C)C
Mol. weight [g/mol]: 212.07

Physical Properties

Property code	Value	Unit	Source
gf	52.88	kJ/mol	Joback Method
hf	-100.86	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	37.55	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.856		Crippen Method
mcvol	121.220	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1029.00		NIST Webbook
rinpol	1029.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1170.00		NIST Webbook
tb	428.94	K	Joback Method
tc	639.15	K	Joback Method
tf	185.44	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.69	J/mol×K	428.94	Joback Method
cpg	221.44	J/mol×K	463.97	Joback Method
cpg	232.57	J/mol×K	499.01	Joback Method
cpg	243.11	J/mol×K	534.04	Joback Method
cpg	253.07	J/mol×K	569.08	Joback Method
cpg	262.50	J/mol×K	604.11	Joback Method

cpg	271.40	J/mol×K	639.15	Joback Method
dvisc	0.0182084	Pa×s	185.44	Joback Method
dvisc	0.0051392	Pa×s	226.02	Joback Method
dvisc	0.0021319	Pa×s	266.61	Joback Method
dvisc	0.0011159	Pa×s	307.19	Joback Method
dvisc	0.0006793	Pa×s	347.77	Joback Method
dvisc	0.0004588	Pa×s	388.36	Joback Method
dvisc	0.0003337	Pa×s	428.94	Joback Method

Sources

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=R25580&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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