Pentane, 3-iodo-3-methyl

Inchi: InChI=1S/C6H13I/c1-4-6(3,7)5-2/h4-5H2,1-3H3
InchiKey: CIDZNASUPYMQCG-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CCC(C)(I)CC
Mol. weight [g/mol]: 212.07

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	958.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1179.00		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	266.25	J/mol×K	605.22	Joback Method
cpg	256.82	J/mol×K	569.49	Joback Method
cpg	246.73	J/mol×K	533.77	Joback Method
cpg	235.92	J/mol×K	498.04	Joback Method
cpg	224.35	J/mol×K	462.32	Joback Method
cpg	275.05	J/mol×K	640.95	Joback Method

dvisc	0.0003828	Pa×s	426.59	Joback Method
dvisc	0.0005200	Pa×s	391.80	Joback Method
dvisc	0.0007498	Pa×s	357.01	Joback Method
dvisc	0.0011699	Pa×s	322.23	Joback Method
dvisc	0.0020332	Pa×s	287.44	Joback Method
dvisc	0.0041142	Pa×s	252.65	Joback Method
dvisc	0.0104269	Pa×s	217.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25594&Units=SI
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

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

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