

Pentane, 2-iodo-3-methyl

Inchi:	InChI=1S/C6H13I/c1-4-5(2)6(3)7/h5-6H,4H2,1-3H3
InchiKey:	MHIYXLPYCSGBRG-UHFFFAOYSA-N
Formula:	C6H13I
SMILES:	CCC(C)C(C)I
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
rinpola	1036.00		NIST Webbook
ripola	1177.00		NIST Webbook
tb	428.94	K	Joback Method
tc	639.15	K	Joback Method
tf	185.44	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.69	J/molxK	428.94	Joback Method
cpg	262.50	J/molxK	604.11	Joback Method
cpg	253.07	J/molxK	569.08	Joback Method
cpg	243.11	J/molxK	534.04	Joback Method
cpg	232.57	J/molxK	499.01	Joback Method
cpg	221.44	J/molxK	463.97	Joback Method
cpg	271.40	J/molxK	639.15	Joback Method
dvisc	0.0003337	Paxs	428.94	Joback Method

dvisc	0.0004588	Paxs	388.36	Joback Method
dvisc	0.0006793	Paxs	347.77	Joback Method
dvisc	0.0011159	Paxs	307.19	Joback Method
dvisc	0.0021319	Paxs	266.61	Joback Method
dvisc	0.0051392	Paxs	226.02	Joback Method
dvisc	0.0182084	Paxs	185.44	Joback Method

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=R25562&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
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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