

Pentane, 1-iodo-3,3-dimethyl

Inchi:	InChI=1S/C7H15I/c1-4-7(2,3)5-6-8/h4-6H2,1-3H3
InchiKey:	FYTNBCANGRHTEA-UHFFFAOYSA-N
Formula:	C7H15I
SMILES:	CCC(C)(C)CI
Mol. weight [g/mol]:	226.10

Physical Properties

Property code	Value	Unit	Source
gf	69.02	kJ/mol	Joback Method
hf	-119.69	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
hvap	39.25	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.248		Crippen Method
mvol	135.310	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rmpol	1054.00		NIST Webbook
ripol	1146.00		NIST Webbook
tb	449.47	K	Joback Method
tc	661.08	K	Joback Method
tf	229.13	K	Joback Method
vc	0.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.87	J/molxK	449.47	Joback Method
cpg	265.42	J/molxK	484.74	Joback Method
cpg	278.11	J/molxK	520.01	Joback Method
cpg	289.99	J/molxK	555.27	Joback Method
cpg	301.13	J/molxK	590.54	Joback Method
cpg	311.55	J/molxK	625.81	Joback Method
cpg	321.31	J/molxK	661.08	Joback Method
dvisc	0.0098571	Paxs	229.13	Joback Method

dvisc	0.0038359	Paxs	265.85	Joback Method
dvisc	0.0018770	Paxs	302.58	Joback Method
dvisc	0.0010722	Paxs	339.30	Joback Method
dvisc	0.0006832	Paxs	376.02	Joback Method
dvisc	0.0004717	Paxs	412.75	Joback Method
dvisc	0.0003460	Paxs	449.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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