

Phenol, 3-methyl-6-iodo

Inchi:	InChI=1S/C7H7IO/c1-5-2-3-6(8)7(9)4-5/h2-4,9H,1H3
InchiKey:	SYJGEJGXAKCKSI-UHFFFAOYSA-N
Formula:	C7H7IO
SMILES:	Cc1ccc(I)c(O)c1
Mol. weight [g/mol]:	234.03

Physical Properties

Property code	Value	Unit	Source
gf	14.34	kJ/mol	Joback Method
hf	-63.19	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	56.50	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.305		Crippen Method
mcvol	117.420	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	1257.00		NIST Webbook
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tb	564.98	K	Joback Method
tc	831.06	K	Joback Method
tf	377.37	K	Joback Method
vc	0.373	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.73	J/molxK	564.98	Joback Method
cpg	261.10	J/molxK	786.71	Joback Method
cpg	254.56	J/molxK	742.37	Joback Method
cpg	247.59	J/molxK	698.02	Joback Method
cpg	240.04	J/molxK	653.67	Joback Method
cpg	231.80	J/molxK	609.33	Joback Method
cpg	267.33	J/molxK	831.06	Joback Method
dvisc	0.0000669	Paxs	564.98	Joback Method

dvisc	0.0000994	Paxs	533.71	Joback Method
dvisc	0.0001552	Paxs	502.44	Joback Method
dvisc	0.0002570	Paxs	471.18	Joback Method
dvisc	0.0004574	Paxs	439.91	Joback Method
dvisc	0.0008888	Paxs	408.64	Joback Method
dvisc	0.0019284	Paxs	377.37	Joback Method

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=R632618&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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