Phenol, 2-methyl-6-iodo

Inchi: InChI=1S/C7H7IO/c1-5-3-2-4-6(8)7(5)9/h2-4,9H,1H3
InchiKey: GZZUGNNHSZONTO-UHFFFAOYSA-N
Formula: C7H7IO
SMILES: Cc1cccc(I)c1O
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	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
tb	564.98	K	Joback Method
tc	831.06	K	Joback Method
tf	377.37	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.73	J/mol×K	564.98	Joback Method
cpg	231.80	J/mol×K	609.33	Joback Method
cpg	240.04	J/mol×K	653.67	Joback Method
cpg	247.59	J/mol×K	698.02	Joback Method
cpg	254.56	J/mol×K	742.37	Joback Method
cpg	261.10	J/mol×K	786.71	Joback Method
cpg	267.33	J/mol×K	831.06	Joback Method
dvisc	0.0019284	Pa×s	377.37	Joback Method

dvisc	0.0008888	Pa×s	408.64	Joback Method
dvisc	0.0004574	Pa×s	439.91	Joback Method
dvisc	0.0002570	Pa×s	471.18	Joback Method
dvisc	0.0001552	Pa×s	502.44	Joback Method
dvisc	0.0000994	Pa×s	533.71	Joback Method
dvisc	0.0000669	Pa×s	564.98	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=R632292&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