3-Iodophenol, isoBOC

Inchi: InChI=1S/C11H13IO3/c1-8(2)7-14-11(13)15-10-5-3-4-9(12)6-10/h3-6,8H,7H2,1-2H3
InchiKey: BORBKNSEZWJISD-UHFFFAOYSA-N
Formula: C11H13IO3
SMILES: CC(C)COC(=O)Oc1cccc(I)c1
Mol. weight [g/mol]: 320.12

Physical Properties

Property code	Value	Unit	Source
gf	-138.72	kJ/mol	Joback Method
hf	-350.74	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	63.57	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.463		Crippen Method
mcvol	181.220	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	674.15	K	Joback Method
tc	912.43	K	Joback Method
tf	390.12	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.27	J/mol×K	674.15	Joback Method
cpg	433.35	J/mol×K	713.86	Joback Method
cpg	445.49	J/mol×K	753.58	Joback Method
cpg	456.72	J/mol×K	793.29	Joback Method
cpg	467.04	J/mol×K	833.00	Joback Method
cpg	476.49	J/mol×K	872.71	Joback Method
cpg	485.07	J/mol×K	912.43	Joback Method
dvisc	0.0014397	Pa×s	390.12	Joback Method

dvisc	0.0007795	Pa×s	437.46	Joback Method
dvisc	0.0004758	Pa×s	484.80	Joback Method
dvisc	0.0003170	Pa×s	532.13	Joback Method
dvisc	0.0002258	Pa×s	579.47	Joback Method
dvisc	0.0001692	Pa×s	626.81	Joback Method
dvisc	0.0001321	Pa×s	674.15	Joback Method

Sources

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=R235133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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