2-Isopropoxyphenol

Other names:	Phenol, 2-(1-methylethoxy)-
	o-Isopropoxyphenol
	Phenol, 2-isopropoxy
Inchi:	InChI=1S/C9H12O2/c1-7(2)11-9-6-4-3-5-8(9)10/h3-7,10H,1-2H3
InchiKey:	ZNCUUYCDKVNVJH-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(C)Oc1ccccc1O
Mol. weight [g/mol]:	152.19
CAS:	4812-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-124.75	kJ/mol	Joback Method
hf	-307.37	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.179		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	534.60	K	Joback Method
tc	759.25	K	Joback Method
tf	336.56	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.61	J/mol×K	534.60	Joback Method
cpg	347.47	J/mol×K	721.81	Joback Method
cpg	337.55	J/mol×K	684.37	Joback Method
cpg	326.97	J/mol×K	646.93	Joback Method
cpg	315.66	J/mol×K	609.48	Joback Method
cpg	303.56	J/mol×K	572.04	Joback Method

cpg	356.79	J/mol×K	759.25	Joback Method
dvisc	0.0000510	Pa×s	534.60	Joback Method
dvisc	0.0000820	Pa×s	501.59	Joback Method
dvisc	0.0001411	Pa×s	468.59	Joback Method
dvisc	0.0002636	Pa×s	435.58	Joback Method
dvisc	0.0005456	Pa×s	402.57	Joback Method
dvisc	0.0012858	Pa×s	369.57	Joback Method
dvisc	0.0035849	Pa×s	336.56	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=C4812208&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume