Isopropylphenol

Other names: Phenol, (1-methylethyl)-
Inchi: InChI=1S/C9H12O/c1-7(2)8-3-5-9(10)6-4-8/h3-7,10H,1-2H3
InchiKey: YQUQWHNMBPIWGK-UHFFFAOYSA-N
Formula: C9H12O
SMILES: CC(C)c1ccc(O)cc1
Mol. weight [g/mol]: 136.19
CAS: 25168-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-19.75	kJ/mol	Joback Method
hf	-175.15	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.516		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	512.18	K	Joback Method
tc	739.56	K	Joback Method
tf	314.33	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.53	J/mol×K	512.18	Joback Method
cpg	325.34	J/mol×K	701.66	Joback Method
cpg	315.38	J/mol×K	663.76	Joback Method
cpg	304.71	J/mol×K	625.87	Joback Method
cpg	293.23	J/mol×K	587.97	Joback Method
cpg	280.87	J/mol×K	550.08	Joback Method
cpg	334.65	J/mol×K	739.56	Joback Method
dvisc	0.0000726	Pa×s	512.18	Joback Method

dvisc	0.0001200	Pa×s	479.21	Joback Method
dvisc	0.0002136	Pa×s	446.23	Joback Method
dvisc	0.0004171	Pa×s	413.25	Joback Method
dvisc	0.0009146	Pa×s	380.28	Joback Method
dvisc	0.0023278	Pa×s	347.31	Joback Method
dvisc	0.0072081	Pa×s	314.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25168063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume