

p-Isopropenylphenol

Other names:	Phenol, 4-(1-methylethenyl)
Inchi:	InChI=1S/C9H10O/c1-7(2)8-3-5-9(10)6-4-8/h3-6,10H,1H2,2H3
InchiKey:	JAGRUUPXPPLSRX-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	<chem>C=C(C)c1ccc(O)cc1</chem>
Mol. weight [g/mol]:	134.18
CAS:	4286-23-1

Physical Properties

Property code	Value	Unit	Source
gf	61.98	kJ/mol	Joback Method
hf	-54.23	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	50.33	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.425		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1296.00		NIST Webbook
tb	509.18	K	Joback Method
tc	740.94	K	Joback Method
tf	313.61	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.08	J/molxK	509.18	Joback Method
cpg	261.48	J/molxK	547.81	Joback Method
cpg	272.90	J/molxK	586.43	Joback Method
cpg	283.42	J/molxK	625.06	Joback Method
cpg	293.16	J/molxK	663.69	Joback Method
cpg	302.20	J/molxK	702.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4286231&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
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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