Phenol, 4-isopropyl-2-methyl (Isocarvacrol)

Inchi: InChI=1S/C10H14O/c1-7(2)9-4-5-10(11)8(3)6-9/h4-7,11H,1-3H3
InchiKey: WYXXLXHHWYNKJF-UHFFFAOYSA-N
Formula: C10H14O
SMILES: Cc1cc(C(C)C)ccc1O
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	-20.96	kJ/mol	Joback Method
hf	-207.26	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	53.42	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.824		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
ripol	2221.00		NIST Webbook
tb	540.04	K	Joback Method
tc	764.51	K	Joback Method
tf	338.12	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.65	J/mol×K	540.04	Joback Method
cpg	372.56	J/mol×K	727.10	Joback Method
cpg	361.90	J/mol×K	689.69	Joback Method
cpg	350.56	J/mol×K	652.28	Joback Method
cpg	338.45	J/mol×K	614.86	Joback Method
cpg	325.50	J/mol×K	577.45	Joback Method
cpg	382.61	J/mol×K	764.51	Joback Method
dvisc	0.0000535	Pa×s	540.04	Joback Method
dvisc	0.0000853	Pa×s	506.39	Joback Method

dvisc	0.0001452	Pa×s	472.73	Joback Method
dvisc	0.0002681	Pa×s	439.08	Joback Method
dvisc	0.0005484	Pa×s	405.43	Joback Method
dvisc	0.0012767	Pa×s	371.77	Joback Method
dvisc	0.0035167	Pa×s	338.12	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R610158&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume