4-Isopropyl-2-methylphenol

Other names: Phenol, 2-methyl-4-(1-methylethyl)-
Isocarvacrol
4-isopropyl-m-cresol
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
CAS: 1740-97-2

Physical Properties

Property code	Value	Unit	Source
chl	-5640.00 ± 10.00	kJ/mol	NIST Webbook
chl	-5653.00	kJ/mol	NIST Webbook
gf	-20.96	kJ/mol	Joback Method
hf	-206.80	kJ/mol	NIST Webbook
hfl	-280.00	kJ/mol	NIST Webbook
hfus	17.57	kJ/mol	Joback Method
hvap	77.74	kJ/mol	NIST Webbook
hvap	56.00 ± 3.00	kJ/mol	NIST Webbook
hvap	73.20	kJ/mol	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.824		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
ripol	2205.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2221.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2221.00		NIST Webbook
ripol	2221.00		NIST Webbook
ripol	2221.00		NIST Webbook
ripol	2221.00		NIST Webbook
tb	506.15 ± 4.00	K	NIST Webbook
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	382.61	J/mol×K	764.51	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	311.65	J/mol×K	540.04	Joback Method
dvisc	0.0035167	Pa×s	338.12	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
hvapt	59.80	kJ/mol	442.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.20	K	0.40	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1740972&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume