Phenol, 4-methyl-2-(1-methylethyl)-

Other names: 2-Isopropyl-4-methylphenol
4-Methyl-2-isopropylphenol (Isothymol)
2-isopropyl-p-cresol
Inchi: InChI=1S/C10H14O/c1-7(2)9-6-8(3)4-5-10(9)11/h4-7,11H,1-3H3
InchiKey: DSTPUJAJSXTJHM-UHFFFAOYSA-N
Formula: C10H14O
SMILES: Cc1ccc(O)c(C(C)C)c1
Mol. weight [g/mol]: 150.22
CAS: 4427-56-9

Physical Properties

Property code	Value	Unit	Source
chl	-5661.00	kJ/mol	NIST Webbook
gf	-20.96	kJ/mol	Joback Method
hf	-198.40	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	81.60	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
rinpol	1262.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2179.00		NIST Webbook
tb	507.65 ± 4.00	K	NIST Webbook
tc	764.51	K	Joback Method
tf	308.15 ± 2.00	K	NIST Webbook
tf	310.15 ± 2.00	K	NIST Webbook
tf	306.65 ± 2.00	K	NIST Webbook
tf	309.65 ± 2.00	K	NIST Webbook
tf	309.15 ± 2.00	K	NIST Webbook
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	325.50	J/mol×K	577.45	Joback Method
cpg	338.45	J/mol×K	614.86	Joback Method
cpg	350.56	J/mol×K	652.28	Joback Method
cpg	361.90	J/mol×K	689.69	Joback Method
cpg	372.56	J/mol×K	727.10	Joback Method
cpg	382.61	J/mol×K	764.51	Joback Method
dvisc	0.0035167	Pa×s	338.12	Joback Method
dvisc	0.0012767	Pa×s	371.77	Joback Method
dvisc	0.0005484	Pa×s	405.43	Joback Method
dvisc	0.0002681	Pa×s	439.08	Joback Method
dvisc	0.0001452	Pa×s	472.73	Joback Method
dvisc	0.0000853	Pa×s	506.39	Joback Method
dvisc	0.0000535	Pa×s	540.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4427569&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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