Phenol, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, (R)-

Other names: (R)-2-Methyl-5-(6-methylhept-5-en-2-yl)phenol
o-Cresol, 5-(1,5-dimethyl-4-hexenyl)-, (-)-
Xanthorrhizol
Phenol, 5-[(1R)-1,5-dimethyl-4-hexen-1-yl]-2-methyl-
Phenol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-2-methyl-
(-)-Xanthorrhizol
(-)-Xanthorrizol
(R)-(-)-Xanthorrhizol
(R)-(-)-Xanthorrizol
(R)-5-(1,5-dimethyl-4-hexenyl)-o-cresol

Inchi: InChI=1S/C15H22O/c1-11(2)6-5-7-12(3)14-9-8-13(4)15(16)10-14/h6,8-10,12,16H,5,7H2,

InchiKey: FKWGCEDRLNNZOZ-LBPRGKRZSA-N

Formula: C15H22O

SMILES: CC(C)=CCCC(C)c1ccc(C)c(O)c1

Mol. weight [g/mol]: 218.33

CAS: 30199-26-9

Physical Properties

Property code	Value	Unit	Source
gf	92.81	kJ/mol	Joback Method
hf	-203.03	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	64.59	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.551		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1749.00		NIST Webbook

rinpol	1754.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1730.00		NIST Webbook
ripol	2674.00		NIST Webbook
tb	658.48	K	Joback Method
tc	876.37	K	Joback Method
tf	375.43	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.73	J/mol×K	658.48	Joback Method
cpg	552.43	J/mol×K	694.79	Joback Method
cpg	568.15	J/mol×K	731.11	Joback Method
cpg	582.99	J/mol×K	767.42	Joback Method
cpg	597.04	J/mol×K	803.74	Joback Method
cpg	610.41	J/mol×K	840.05	Joback Method
cpg	623.20	J/mol×K	876.37	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30199269&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume