Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-

Other names:	Phenol, 2,4-bis(1,1-dimethylethyl)-6-methyl-
	6-Methyl-2,4-di-tert-butyl-phenol
	4,6-Di-(1,1-dimethylethyl)-2-methyl phenol
	2,4-Di-t-butyl-6-methylphenol
	4,6-di-tert-butyl-o-cresol
Inchi:	InChI=1S/C15H24O/c1-10-8-11(14(2,3)4)9-12(13(10)16)15(5,6)7/h8-9,16H,1-7H3
InchiKey:	ZZZRZBIPCKQDQR-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	Cc1cc(C(C)(C)C)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	220.35
CAS:	616-55-7

Physical Properties

Property code	Value	Unit	Source
gf	19.63	kJ/mol	Joback Method
hf	-334.15	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	63.01	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.296		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
ripol	1904.00		NIST Webbook
ripol	1904.00		NIST Webbook
tb	542.20	K	NIST Webbook
tc	880.13	K	Joback Method
tf	426.83	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.55	J/mol×K	653.40	Joback Method
cpg	580.43	J/mol×K	691.19	Joback Method

cpg	597.12	J/mol×K	728.98	Joback Method
cpg	612.75	J/mol×K	766.77	Joback Method
cpg	627.45	J/mol×K	804.56	Joback Method
cpg	641.37	J/mol×K	842.35	Joback Method
cpg	654.63	J/mol×K	880.13	Joback Method
dvisc	0.0006069	Pa×s	426.83	Joback Method
dvisc	0.0002505	Pa×s	464.59	Joback Method
dvisc	0.0001181	Pa×s	502.35	Joback Method
dvisc	0.0000618	Pa×s	540.12	Joback Method
dvisc	0.0000352	Pa×s	577.88	Joback Method
dvisc	0.0000215	Pa×s	615.64	Joback Method
dvisc	0.0000139	Pa×s	653.40	Joback Method
hvapt	59.80	kJ/mol	451.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C616557&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

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
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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume