Phenol, 2,6-bis(1,1-dimethylpropyl)-4-methyl-

Other names:	2,6-Di-tert-amyl-4-cresol
	2,6-Bis-(1,1-dimethyl-propyl)-4-methyl-phenol
	4-Methyl-2,6-di-tert-pentylphenol
Inchi:	InChI=1S/C17H28O/c1-8-16(4,5)13-10-12(3)11-14(15(13)18)17(6,7)9-2/h10-11,18H,8-9H
InchiKey:	SOASHAVJCWKTKL-UHFFFAOYSA-N
Formula:	C17H28O
SMILES:	CCC(C)(C)c1cc(C)cc(C(C)(C)CC)c1O
Mol. weight [g/mol]:	248.40
CAS:	56103-67-4

Physical Properties

Property code	Value	Unit	Source
gf	36.47	kJ/mol	Joback Method
hf	-375.43	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	67.46	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	5.076		Crippen Method
mcvol	232.500	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	699.16	K	Joback Method
tc	918.04	K	Joback Method
tf	449.37	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.74	J/mol×K	918.04	Joback Method
cpg	670.02	J/mol×K	699.16	Joback Method
cpg	688.50	J/mol×K	735.64	Joback Method
cpg	705.86	J/mol×K	772.12	Joback Method
cpg	722.24	J/mol×K	808.60	Joback Method
cpg	737.76	J/mol×K	845.08	Joback Method

cpg	752.55	J/mol×K	881.56	Joback Method
dvisc	0.0000087	Pa×s	699.16	Joback Method
dvisc	0.0004047	Pa×s	449.37	Joback Method
dvisc	0.0001625	Pa×s	491.00	Joback Method
dvisc	0.0000753	Pa×s	532.63	Joback Method
dvisc	0.0000390	Pa×s	574.26	Joback Method
dvisc	0.0000221	Pa×s	615.90	Joback Method
dvisc	0.0000134	Pa×s	657.53	Joback Method
hvapt	65.90	kJ/mol	497.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56103674&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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