3,5-di-tert-Butyl-4-hydroxyanisole

Other names:	3,5-di-t-Butyl-4-hydroxyanisole
	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy-
	Phenol, 2,6-di-tert-butyl-4-methoxy-
	Topanol 354
	2,6-Bis(1,1-dimethylethyl)-4-methoxyphenol
	2,6-Di-tert-butyl-4-methoxyphenol
	Phenol, 4-methoxy, 2,6-bis-(1,1-dimethylethyl)
Inchi:	InChI=1S/C15H24O2/c1-14(2,3)11-8-10(17-7)9-12(13(11)16)15(4,5)6/h8-9,16H,1-7H3
InchiKey:	SLUKQUGVTITNSY-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	COc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	236.35
CAS:	489-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-85.37	kJ/mol	Joback Method
hf	-466.37	kJ/mol	Joback Method
hfus	20.01	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.996		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1527.00		NIST Webbook
tb	675.82	K	Joback Method
tc	899.57	K	Joback Method
tf	449.06	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.82	J/mol×K	899.57	Joback Method

cpg	589.88	J/mol×K	675.82	Joback Method
cpg	607.26	J/mol×K	713.11	Joback Method
cpg	623.52	J/mol×K	750.40	Joback Method
cpg	638.80	J/mol×K	787.69	Joback Method
cpg	653.20	J/mol×K	824.99	Joback Method
cpg	666.84	J/mol×K	862.28	Joback Method
dvisc	0.0000096	Pa×s	675.82	Joback Method
dvisc	0.0003388	Pa×s	449.06	Joback Method
dvisc	0.0001485	Pa×s	486.85	Joback Method
dvisc	0.0000733	Pa×s	524.65	Joback Method
dvisc	0.0000398	Pa×s	562.44	Joback Method
dvisc	0.0000233	Pa×s	600.23	Joback Method
dvisc	0.0000146	Pa×s	638.03	Joback Method
hfust	26.90	kJ/mol	374.40	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C489010&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume