2,6-Di-tert-butyl-4-methoxyphenol

Other names: 2,6-Bis(1,1-dimethylethyl)-4-methoxyphenol
2,6-Di-tert-butyl-4-methoxyphenol
3,5-di-t-Butyl-4-hydroxyanisole
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy-
Phenol, 2,6-di-tert-butyl-4-methoxy-
Phenol, 4-methoxy, 2,6-bis-(1,1-dimethylethyl)
Topanol 354

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]: 236.36

Physical Properties

Property code	Value	Unit	Source
hf	-415.95	kJ/mol	Cheméo Relay (1.0)
hfus	20.01	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Cheméo Relay (1.0)
ie	7.68	eV	Cheméo Relay (1.0)
log10ws	-4.67		Cheméo Relay (1.0)
logp	3.996		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
rinpol	1527.00		NIST Webbook
tb	553.67	K	Cheméo Relay (1.0)
tf	361.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	679.82	J/mol×K	899.57	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
dvisc	0.0000096	Pa×s	675.82	Joback Method
hfust	26.90	kJ/mol	374.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C489010&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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