

1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl)-

Other names:	1,4-Dihydroxy-2,5-di-tert-butylbenzene 2,5-Bis(1,1-dimethylethyl)-1,4-benzenediol 2,5-Di-tert-butyl-1,4-benzohydroquinone 2,5-Di-tert-butyl-1,4-dihydroxybenzene 2,5-Di-tert-butyl-1,4-hydroquinone 2,5-Di-tert-butylbenzene-1,4-diol 2,5-Di-tert-butylquinol 2,5-di-t-Butylhydroquinone 2,5-di-tert-butylhydroquinone Antage DBH DBH DTBHQ Di-t-butylhydroquinone Dibug Dybug Eastman DTBHQ Hydroquinone, 2,5-di-tert-butyl- NSC 11 Naugard 451 Nocrac NS 7 Nonflex Alba Santovar O
Inchi:	InChI=1S/C14H22O2/c1-13(2,3)9-7-12(16)10(8-11(9)15)14(4,5)6/h7-8,15-16H,1-6H3
InchiKey:	JZODKRWQWUWGCD-UHFFFAOYSA-N
Formula:	C14H22O2
SMILES:	CC(C)(C)c1cc(O)c(C(C)(C)C)cc1O
Mol. weight [g/mol]:	222.32
CAS:	88-58-4

Physical Properties

Property code	Value	Unit	Source
gf	-133.78	kJ/mol	Joback Method
hf	-479.35	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	73.13	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method

logp	3.693		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1457.00		NIST Webbook
tb	706.16	K	Joback Method
tc	944.46	K	Joback Method
tf	514.76	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.27	J/mol×K	706.16	Joback Method
cpg	636.41	J/mol×K	904.74	Joback Method
cpg	623.37	J/mol×K	865.02	Joback Method
cpg	610.05	J/mol×K	825.31	Joback Method
cpg	596.24	J/mol×K	785.59	Joback Method
cpg	581.71	J/mol×K	745.88	Joback Method
cpg	649.38	J/mol×K	944.46	Joback Method
dvisc	0.0000010	Pa×s	706.16	Joback Method
dvisc	0.0000016	Pa×s	674.26	Joback Method
dvisc	0.0000028	Pa×s	642.36	Joback Method
dvisc	0.0000049	Pa×s	610.46	Joback Method
dvisc	0.0000094	Pa×s	578.56	Joback Method
dvisc	0.0000192	Pa×s	546.66	Joback Method
dvisc	0.0000430	Pa×s	514.76	Joback Method

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=C88584&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

**Solubility of
2,5-Di-tert-butylhydroquinone and
Process Design for Its Purification
Using Crystallization:**

<https://www.doi.org/10.1021/je501049c>

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
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

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