

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

Other names:	Hydroquinone, 2,5-di-tert-pentyl-Santovar A 2,5-Bis(1,1-dimethylpropyl)-1,4-benzenediol 2,5-Bis(1,1-dimethylpropyl)hydroquinone 2,5-Di-tert-amylhydroquinone 2,5-Di-tert-pentylhydroquinone Hydroquinone, 2,5-di-tert-amyl-Santouar A USAF B-21 Hydroquinone, 2,5-di-t-pentyl-2,5-Di-tert-amylbenzene-1,4-diol 2,5-Di-t-amylhydroquinone 2,5-Di-tert-pentylbenzene-1,4-diol 2,5-Di-t-pentylhydroquinone 2,5-Di-t-amyl-p-hydroquinone Lowinox AH25 Antage DAH DAHQ NSC 455
Inchi:	InChI=1S/C16H26O2/c1-7-15(3,4)11-9-14(18)12(10-13(11)17)16(5,6)8-2/h9-10,17-18H,7
InchiKey:	CZNRFEXEPBITDS-UHFFFAOYSA-N
Formula:	C16H26O2
SMILES:	CCC(C)(C)c1cc(O)c(C(C)(C)CC)cc1O
Mol. weight [g/mol]:	250.38
CAS:	79-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-116.94	kJ/mol	Joback Method
hf	-520.63	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	4.473		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
tb	751.92	K	Joback Method

tc	981.44	K	Joback Method
tf	537.30	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.63	J/mol×K	751.92	Joback Method
cpg	689.99	J/mol×K	790.17	Joback Method
cpg	705.56	J/mol×K	828.43	Joback Method
cpg	720.54	J/mol×K	866.68	Joback Method
cpg	735.14	J/mol×K	904.94	Joback Method
cpg	749.54	J/mol×K	943.19	Joback Method
cpg	763.94	J/mol×K	981.44	Joback Method
dvisc	0.0000258	Pa×s	537.30	Joback Method
dvisc	0.0000111	Pa×s	573.07	Joback Method
dvisc	0.0000052	Pa×s	608.84	Joback Method
dvisc	0.0000027	Pa×s	644.61	Joback Method
dvisc	0.0000015	Pa×s	680.38	Joback Method
dvisc	0.0000009	Pa×s	716.15	Joback Method
dvisc	0.0000005	Pa×s	751.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79743&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
h_{vap}:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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