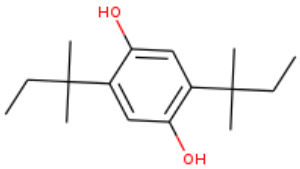
1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-

Other names: 2,5-Bis(1,1-dimethylpropyl)-1,4-benzenediol; 2,5-Bis(1,1-dimethylpropyl)hydroquinone; 2,5-Di-t-amyl-p-hydroquinone; 2,5-Di-t-amylhydroquinone; 2,5-Di-t-pentylhydroquinone; 2,5-Di-tert-amylbenzene-1,4-diol; 2,5-Di-tert-amylhydroquinone; 2,5-Di-tert-pentylbenzene-1,4-diol; 2,5-Di-tert-pentylhydroquinone; Antage DAH; DAHQ; Hydroquinone, 2,5-di-t-pentyl-; Hydroquinone, 2,5-di-tert-amyl-; Hydroquinone, 2,5-di-tert-pentyl-; Lowinox AH25; NSC 455; Santouar A; Santovar A; USAF B-21.



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,7-8H2,1-6H3

InChI Key: CZNRFEXEPBITDS-UHFFFAOYSA-N

Formula: C16H26O2

SMILES: CCC(C)(C)c1cc(O)c(C(C)(C)CC)cc1O

Molecular Weight: 250.38

CAS: 79-74-3

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-116.94	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-520.63	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.59	kJ/mol	Joback Method
$\Delta_{vap} H°$	77.58	kJ/mol	Joback Method
$logP_{oct/wat}$	4.47		Crippen Method
P_c	2263.26	kPa	Joback Method
T_{boil}	751.92	K	Joback Method
T_c	981.44	K	Joback Method
T_{fus}	537.30	K	Joback Method
V_c	0.73	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	673.63	J/mol×K	751.92	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.00	Pa×s	751.92	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/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,7-8H2,1-6H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).

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