4-t-Butylbenzene-1,2-diol

Other names: 1,2-Benzenediol, 4-(1,1-dimethylethyl)-
1,2-Dihydroxy-4-tert-butylbenzene
4-TBC
4-t-Butyl-1,2-benzenediol
4-t-Butylcatechol
4-t-Butylpyrocatechol
4-tert-Butyl-1,2-benzenediol
4-tert-Butyl-1,2-dihydroxybenzene
4-tert-Butylcatechin
4-tert-Butylcatechol
4-tert-Butylpyrocatechol
4-tert-Butylpyrokatechin
NSC 5310
Pyrocatechol, 4-tert-butyl-
Synox TBC
p-t-Butyl catechol
p-t-Butylpyrocatechol
p-tert-Butylcatechol
p-tert-Butylpyrocatechol

Inchi: InChI=1S/C10H14O2/c1-10(2,3)7-4-5-8(11)9(12)6-7/h4-6,11-12H,1-3H3

InchiKey: XESZUVZBAMCAEJ-UHFFFAOYSA-N

Formula: C10H14O2

SMILES: CC(C)(C)c1ccc(O)c(O)c1

Mol. weight [g/mol]: 166.22

CAS: 98-29-3

Physical Properties

Property code	Value	Unit	Source
chs	-5461.90 ± 0.90	kJ/mol	NIST Webbook
hf	-374.70 ± 2.10	kJ/mol	NIST Webbook
hfs	-474.00 ± 1.60	kJ/mol	NIST Webbook
hfus	19.85	kJ/mol	Joback Method
hsub	99.30	kJ/mol	NIST Webbook
hsub	99.30 ± 1.40	kJ/mol	NIST Webbook
hsub	99.20 ± 0.90	kJ/mol	NIST Webbook
hsub	99.30 ± 1.40	kJ/mol	NIST Webbook
hvap	96.50 ± 2.80	kJ/mol	NIST Webbook

ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-2.40		Cheméo Relay (1.0)
logp	2.395		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3700.00 ± 300.00	kPa	NIST Webbook
rhoc	297.53 ± 14.96	kg/m3	NIST Webbook
rinpol	1493.00		NIST Webbook
tb	558.20	K	NIST Webbook
tc	775.00 ± 6.00	K	NIST Webbook
tf	373.43	K	Cheméo Relay (1.0)
tt	327.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.71	J/mol×K	612.89	Joback Method
cpg	429.06	J/mol×K	856.37	Joback Method
cpg	419.64	J/mol×K	815.79	Joback Method
cpg	409.96	J/mol×K	775.21	Joback Method
cpg	399.81	J/mol×K	734.63	Joback Method
cpg	389.01	J/mol×K	694.05	Joback Method
cpg	377.38	J/mol×K	653.47	Joback Method
dvisc	0.0000131	Pa×s	560.17	Joback Method
dvisc	0.0000048	Pa×s	612.89	Joback Method
dvisc	0.0000078	Pa×s	586.53	Joback Method
dvisc	0.0001976	Pa×s	454.74	Joback Method
dvisc	0.0000234	Pa×s	533.82	Joback Method
dvisc	0.0000442	Pa×s	507.46	Joback Method
dvisc	0.0000897	Pa×s	481.10	Joback Method
hfust	15.10	kJ/mol	330.40	NIST Webbook
hsubt	98.70 ± 0.90	kJ/mol	313.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58862e+01

Coeff. B	-5.21116e+03
Coeff. C	-9.57200e+01
Temperature range (K), min.	429.80
Temperature range (K), max.	588.51

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98293&Units=SI

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

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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation 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
pc: Critical Pressure
pvap: Vapor pressure
rhoc: Critical density
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

tt: Triple Point Temperature