Alpha,alpha,alpha',alpha'-tetramethyl-1,4-benzene

Other names: «alpha»,«alpha»'-Dihydroxy-p-diisopropylbenzene
1,4-Benzenedimethanol, «alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-
alpha,alpha,alpha',alpha'-Tetramethyl-1,4-benzenedimethanol
«alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-p-xylene-«alpha»,«alpha»'-diol
Inchi: InChI=1S/C12H18O2/c1-11(2,13)9-5-7-10(8-6-9)12(3,4)14/h5-8,13-14H,1-4H3
InchiKey: LEARFTRDZQQTDN-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(C)(O)c1ccc(C(C)(C)O)cc1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
chs	-6751.60 ± 1.40	kJ/mol	NIST Webbook
hf	-416.69	kJ/mol	Cheméo Relay (1.0)
hfs	-543.00 ± 1.50	kJ/mol	NIST Webbook
hfus	13.84	kJ/mol	Joback Method
hsub	136.80 ± 2.80	kJ/mol	NIST Webbook
hvap	97.16	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	2.141		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	526.02	K	Cheméo Relay (1.0)
tc	775.19	K	Cheméo Relay (1.0)
tf	395.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.07	J/mol×K	683.52	Joback Method
cpg	480.04	J/mol×K	716.49	Joback Method
cpg	491.22	J/mol×K	749.46	Joback Method
cpg	501.68	J/mol×K	782.42	Joback Method

cpg	511.48	J/mol×K	815.39	Joback Method
cpg	520.68	J/mol×K	848.36	Joback Method
cpg	529.35	J/mol×K	881.33	Joback Method
dvisc	0.0036683	Pa×s	390.42	Joback Method
dvisc	0.0008008	Pa×s	439.27	Joback Method
dvisc	0.0002371	Pa×s	488.12	Joback Method
dvisc	0.0000876	Pa×s	536.97	Joback Method
dvisc	0.0000382	Pa×s	585.82	Joback Method
dvisc	0.0000189	Pa×s	634.67	Joback Method
dvisc	0.0000104	Pa×s	683.52	Joback Method

Sources

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=C2948461&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hsub: Enthalpy of sublimation at standard conditions
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point