5-tert-Butylpyrogallol

Inchi: InChI=1S/C10H14O3/c1-10(2,3)6-4-7(11)9(13)8(12)5-6/h4-5,11-13H,1-3H3
InchiKey: HCNISNCKPIVZDX-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: CC(C)(C)c1cc(O)c(O)c(O)c1
Mol. weight [g/mol]: 182.22
CAS: 20481-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-315.29	kJ/mol	Joback Method
hf	-553.88	kJ/mol	Joback Method
hfus	25.63	kJ/mol	Joback Method
hvap	77.88	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	2.101		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	5243.40	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	693.51	K	Joback Method
tc	944.94	K	Joback Method
tf	566.46	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.26	J/mol×K	693.51	Joback Method
cpg	419.07	J/mol×K	735.41	Joback Method
cpg	429.34	J/mol×K	777.32	Joback Method
cpg	439.31	J/mol×K	819.22	Joback Method
cpg	449.26	J/mol×K	861.13	Joback Method
cpg	459.45	J/mol×K	903.03	Joback Method
cpg	470.15	J/mol×K	944.94	Joback Method

dvisc	0.0000036	Pa×s	566.46	Joback Method
dvisc	0.0000020	Pa×s	587.63	Joback Method
dvisc	0.0000012	Pa×s	608.81	Joback Method
dvisc	0.0000007	Pa×s	629.99	Joback Method
dvisc	0.0000004	Pa×s	651.16	Joback Method
dvisc	0.0000003	Pa×s	672.34	Joback Method
dvisc	0.0000002	Pa×s	693.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20481178&Units=SI

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