4,6-di-t-Butylpyrogallol

Other names: 4,6-di-tert-Butylpyrogallol
Inchi: InChI=1S/C14H22O3/c1-13(2,3)8-7-9(14(4,5)6)11(16)12(17)10(8)15/h7,15-17H,1-6H3
InchiKey: NRVDOWRFIAEMPS-UHFFFAOYSA-N
Formula: C14H22O3
SMILES: CC(C)(C)c1cc(C(C)(C)C)c(O)c(O)c1O
Mol. weight [g/mol]: 238.32
CAS: 3934-77-8

Physical Properties

Property code	Value	Unit	Source
gf	-288.40	kJ/mol	Joback Method
hf	-656.66	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	86.15	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	3.398		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	786.78	K	Joback Method
tc	1031.69	K	Joback Method
tf	626.48	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.51	J/mol×K	786.78	Joback Method
cpg	629.72	J/mol×K	827.60	Joback Method
cpg	643.67	J/mol×K	868.42	Joback Method
cpg	657.64	J/mol×K	909.24	Joback Method
cpg	671.92	J/mol×K	950.06	Joback Method
cpg	686.79	J/mol×K	990.87	Joback Method
cpg	702.55	J/mol×K	1031.69	Joback Method
dvisc	0.0000007	Pa×s	626.48	Joback Method

dvisc	0.0000004	Pa×s	653.20	Joback Method
dvisc	0.0000002	Pa×s	679.91	Joback Method
dvisc	0.0000001	Pa×s	706.63	Joback Method
dvisc	7.6925966e-08	Pa×s	733.35	Joback Method
dvisc	4.8484705e-08	Pa×s	760.06	Joback Method
dvisc	3.1531973e-08	Pa×s	786.78	Joback Method

Sources

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=C3934778&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume