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]: 238.33

Physical Properties

Property code	Value	Unit	Source
hf	-617.18	kJ/mol	Cheméo Relay (1.0)
hfus	28.19	kJ/mol	Joback Method
hvap	118.65	kJ/mol	Cheméo Relay (1.0)
ie	7.81	eV	Cheméo Relay (1.0)
logp	3.398		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
tb	567.54	K	Cheméo Relay (1.0)
tf	389.61	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3934778&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point