Nordihydroguaiaretic acid

Other names: 1,2-Benzenediol, 4,4'-(2,3-dimethyl-1,4-butanediyl)bis-
Pyrocatechol, 4,4'-(2,3-dimethyltetramethylene)di-
«beta»,«gamma»-Dimethyl-«alpha»,«delta»-bis(3,4-dihydroxyphenyl)butane
Butane, 1,4-bis(3,4-dihydroxyphenyl)-2,3-dimethyl-
Dihydronorguaiaretic acid
Dinorguaiaretic acid, dihydro-
Norguaiaretic acid, dihydro-
NDGA
4,4'-(2,3-Dimethyl-1,4-Butanediyl)bis(pyrocatechol)
4,4'-(2,3-Dimethyltetramethylene)dipyrocatechol
Nordihydroguairaretic acid
2,3-Bis(3,4-dihydroxyphenylmethyl)butane
NSC 4291
1,4-Bis(3,4-dihydroxyphenyl)-2,3-dimethylbutane

Inchi: InChI=1S/C18H22O4/c1-11(7-13-3-5-15(19)17(21)9-13)12(2)8-14-4-6-16(20)18(22)10-14

InchiKey: HCZKYJDFEPMADG-UHFFFAOYSA-N

Formula: C18H22O4

SMILES: CC(Cc1ccc(O)c(O)c1)C(C)Cc1ccc(O)c(O)c1

Mol. weight [g/mol]: 302.36

CAS: 500-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-297.86	kJ/mol	Joback Method
hf	-661.59	kJ/mol	Joback Method
hfus	46.54	kJ/mol	Joback Method
hvap	111.49	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.566		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	986.20	K	Joback Method
tc	1242.87	K	Joback Method
tf	762.34	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.61	J/mol×K	986.20	Joback Method
cpg	908.91	J/mol×K	1200.09	Joback Method
cpg	882.03	J/mol×K	1157.31	Joback Method
cpg	857.63	J/mol×K	1114.53	Joback Method
cpg	835.34	J/mol×K	1071.76	Joback Method
cpg	814.79	J/mol×K	1028.98	Joback Method
cpg	938.63	J/mol×K	1242.87	Joback Method
dvisc	1.5638068e-10	Pa×s	986.20	Joback Method
dvisc	2.5433751e-10	Pa×s	948.89	Joback Method
dvisc	4.3045559e-10	Pa×s	911.58	Joback Method
dvisc	7.6199227e-10	Pa×s	874.27	Joback Method
dvisc	1.4193367e-09	Pa×s	836.96	Joback Method
dvisc	2.8017423e-09	Pa×s	799.65	Joback Method
dvisc	5.9112580e-09	Pa×s	762.34	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=C500389&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