

Guaifenesin

Other names: 1,2-Dihydroxy-3-(2-methoxyphenoxy)propane
1,2-Propanediol, 3-(2-methoxyphenoxy)-
1,2-Propanediol, 3-(o-methoxyphenoxy)-
2-G
2/G
3-(2-Methoxyphenoxy)-1,2-propanediol
3-(o-Methoxyphenoxy)-1,2-propanediol
3-(o-Methoxyphenoxy)-propanediol-1,2
3-o-Methoxyphenoxypropane 1:2-diol
Actifed C
Aeronesin
Amonidren
Amonidrin
Aresol
Breonesin
Bronchol
Calmipan
Colrex expectorant
Cortussin
Creson
Dilyn
Dorassin
Equicol
Flartussin
G 87
GGE
GGG
Gaiamar
Glycerin guaiacolate
Glycerin monoguaiacol ether
Glycero-guaiacol ether
Glycerol guaiacolate
Glycerol mono(2-methoxyphenyl) ether
Glycerol «alpha»-(2-methoxyphenyl) ether
Glycerol «alpha»-(o-methoxyphenyl)ether
Glycerol «alpha»-guaiacyl ether
Glycerol «alpha»-guiacyl ether
Glycerol «alpha»-monoguaiacol ether
Glycerol Â«alphaÂ»-(2-methoxyphenyl) ether
Glycerol Â«alphaÂ»-(o-methoxyphenyl)ether

Glycerol $\hat{\alpha}$ -guaiacyl ether
Glycerol $\hat{\alpha}$ -guiacyl ether
Glycerol $\hat{\alpha}$ -monoguaiacol ether
Glycerol, 1-(2-methoxyphenyl) ether
Glycerol- α -guajakolether
Glycerol- $\hat{\alpha}$ -guajakolether
Glyceryl guaiacol
Glyceryl guaiacol ether
Glyceryl guaiacolate
Glyceryl guaiacolate ether
Glyceryl guaiacyl ether
Glyceryl guaicolate
Glyceryl guiacolate
Glycodex
Glycotuss
Gnaifenesin
Guaia-rom
Guaiacol glycerin ether
Guaiacol glycerol ether
Guaiacol glyceryl ether
Guaiacolglicerinetere
Guaiacolic acid, ester with glycerol
Guaiacuran
Guaiacurane
Guaiacyl glyceryl ether
Guaamar
Guaianesin
Guaicol glycerine ether
Guaicol glyceryl ether
Guaifenesine
Guaiphenesin
Guaiphenesine
Guaiphesin
Guajacol-glycerinaether
Guajacol- α -glycerin-ether
Guajacol- $\hat{\alpha}$ -glycerin-ether
Guajacuran
Guajamar
Guanar
Guayanesin
Guiaphenesin
Gvaja
Hustodil

Hustosil
Hytuss
Metfenossidiolo
Methoxypropanediol
Methphenoxydiol
Metossipropandiolo
Mintosyl
Miocaina
Miocurin
Miorelax
Mucinex
Mucostop
Muskurelax
My 301
Myocain
Myocaine
Myorelax
Myoscain
Myoscaine
Neuroton
Neurotone
Oresol
Oreson
Organidin NR
Propanosedyl
Reduton
Relaxil G
Relaxyl-G
Reorganin
Resil
Respenyl
Respil
Resyl
Ritussin
Robitussin
SL-90
Sirotol
Tenntus
Tenntuss
Tolseron
Tolyn
Trecid
Tulyl

	Tulyl
	XL-90
	o-Methoxyphenyl glyceryl ether
	«alpha»-Glyceryl guaiacol ether
	«alpha»-Glyceryl guaiacolate ether
	Â«alphaÂ»-Glyceryl guaiacol ether
	Â«alphaÂ»-Glyceryl guaiacolate ether
Inchi:	InChI=1S/C10H14O4/c1-13-9-4-2-3-5-10(9)14-7-8(12)6-11/h2-5,8,11-12H,6-7H2,1H3
InchiKey:	HSRJKNPTNIJEKV-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	COc1cccc1OCC(O)CO
Mol. weight [g/mol]:	198.22
CAS:	93-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-349.98	kJ/mol	Joback Method
hf	-598.85	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	0.427		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rmpol	1650.00		NIST Webbook
tb	688.62	K	Joback Method
tc	874.37	K	Joback Method
tf	352.58	K	Aqueous Solubility Prediction Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.54	J/mol×K	688.62	Joback Method
cpg	420.75	J/mol×K	719.58	Joback Method

cpg	430.42	J/molxK	750.54	Joback Method
cpg	439.53	J/molxK	781.49	Joback Method
cpg	448.10	J/molxK	812.45	Joback Method
cpg	456.13	J/molxK	843.41	Joback Method
cpg	463.62	J/molxK	874.37	Joback Method
dvisc	0.0022712	Paxs	392.50	Joback Method
dvisc	0.0005544	Paxs	441.85	Joback Method
dvisc	0.0001797	Paxs	491.21	Joback Method
dvisc	0.0000715	Paxs	540.56	Joback Method
dvisc	0.0000332	Paxs	589.91	Joback Method
dvisc	0.0000174	Paxs	639.27	Joback Method
dvisc	0.0000100	Paxs	688.62	Joback Method

Sources

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C93141&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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