1,2-Propanediol, 3-(2-methoxyphenoxy)-

Other names:

1,2-Dihydroxy-3-(2-methoxyphenoxy)propane
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, 1-(2-methoxyphenyl) ether
Glycerol-«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
Guaiamar
Guaianesin
Guaicol glycerine ether
Guaicol glyceryl ether
Guaifenesine
Guaiphenesin
Guaiphenesine
Guaiphesin
Guajacol-glycerinaether
Guajacol-«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
Tulyn
XL-90
guaifenesin
o-Methoxyphenyl glyceryl ether
«alpha»-Glyceryl guaiacol ether
«alpha»-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: COc1ccccc1OCC(O)CO
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
hfus	22.34	kJ/mol	Joback Method
hvap	104.67	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	0.427		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
rinpol	1650.00		NIST Webbook
tb	614.28	K	Cheméo Relay (1.0)
tf	352.58	K	Aqueous Solubility Prediction 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/mol×K	750.54	Joback Method
cpg	439.53	J/mol×K	781.49	Joback Method
cpg	448.10	J/mol×K	812.45	Joback Method
cpg	456.13	J/mol×K	843.41	Joback Method
cpg	463.62	J/mol×K	874.37	Joback Method
dvisc	0.0022712	Pa×s	392.50	Joback Method
dvisc	0.0005544	Pa×s	441.85	Joback Method
dvisc	0.0001797	Pa×s	491.21	Joback Method
dvisc	0.0000715	Pa×s	540.56	Joback Method
dvisc	0.0000332	Pa×s	589.91	Joback Method
dvisc	0.0000174	Pa×s	639.27	Joback Method
dvisc	0.0000100	Pa×s	688.62	Joback Method

Sources

Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93141&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point