Mephenesin

Other names:

(+/-)-Mephenesin
1,2-Dihydroxy-3-(2-methylphenoxy)propane
1,2-Propanediol, 3-(2-methylphenoxy)-
1,2-Propanediol, 3-(o-tolyloxy)-
1-Ortho-tolylglycerol ether
1-o-Tolylglycerol ether
3-(2-Methylphenoxy)-1,2-propanediol
3-(2-Methylphenoxy)propane-1,2-diol
3-(2-Tolyloxy)-1,2-propanediol
3-(o-Methylphenoxy)-1,2-propanediol
3-(o-Tolyloxy)-1,2-propanediol
3-(o-Tolyloxy)propane-1,2-diol
3-o-Toloxy-1,2-propanediol
A 1141
Ageflex CGE
Anatensin
Anxine
Atensin
Avesyl
Avosyl
Avoxil
Avoxyl
BDH 312
BYK-M 1
Cresodiol
Cresossidiolo
Cresossipropandiolo
Cresoxydiol
Cresoxypropanediol
Curaril
Curarythan
Curythan
Daserd
Daserol
Decontractil
Decontractyl
Diloxol
Dioloxal
Dioloxol
Findolar

Findolor
Glukresin
Glyceryl o-Tolyl ether
Glykresin
Glyotol
Glytol
Halabar
Kinavosyl
Kresoxypropandiol
Lissenphan
Lissephen
Mc 2303
Mefenesina
Mefensina
Memphenesin
Mephate
Mephedan
Mephelor
Mephenesine
Mephensin
Mepherol
Mephesin
Mephin
Mephosal
Mephson
Mervaldin
Mianesina
Miolisina
Moctynol
Myanesin
Myanil
Myanol
Myasin
Myastenin
Mycocuran
Myocaine
Myocuran
Myodetensin
Myodetensine
Myolax
Myolysin
Myopan
Myopen

Myopna
Myosera
Myoserol
Myoten
Myoxane
Myoxyl
Nembusen
Nephelor
Noctynol
Oranixon
Oronixon
Ortol
Prolax
Prolaxin
Proloxin
RP 3602
Relaxant
Relaxar
Relaxil
Relaxyl
Renarcol
Rex regulans
Rhex
Rhex 'hobeino'
Rhex regulans
SQ 1156
Sansdolor
Saserol
Seconesinz
Sinan
Spartoloxin
Spartoloxyn
Spasmolyn
Stilalgin
Temian
Thioxidil
Thoxidil
Tokerol
Tolansin
Tolax
Tolbart
Tolcil
Tolhart

	Tolofren
	Tolosate
	Toloxyn
	Tolserol
	Tolseron
	Tolsil
	Tolsin
	Tolulexin
	Tolulox
	Tolydrin
	Tolynol
	Tolyspaz
	Torulox
	Vitamisin
	Vitascorbol
	Walconesin
	Walko-Nesin
	Xeral
	Xitix
	component of Tolagesic
	o-Cresol glyceryl ether
	o-Cresyl glycerol ether
	o-Cresyl «alpha»-glyceryl ether
	o-Cresyl Â«alphaÂ»-glyceryl ether
	o-Kresol-glycerinaether
	«alpha»,«beta»-Dihydroxy-«gamma»-(2-methylphenoxy)propane
	«alpha»-(o-Tolyl)glyceryl ether
	Â«alphaÂ»,Â«betaÂ»-Dihydroxy-Â«gammaÂ»-(2-methylphenoxy)propane
	Â«alphaÂ»-(o-Tolyl)glyceryl ether
Inchi:	InChI=1S/C10H14O3/c1-8-4-2-3-5-10(8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3
InchiKey:	JWDYCNIAQWPBHD-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	Cc1ccccc1OCC(O)CO
Mol. weight [g/mol]:	182.22
CAS:	59-47-2

Physical Properties

Property code	Value	Unit	Source
gf	-244.98	kJ/mol	Joback Method

hf	-466.63	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Study of Glass Transition Phenomena in the Supercooled Liquid Phase of Methocarbamol, Acetaminophen and Mephensin
hvap	76.17	kJ/mol	Joback Method
log10ws	-1.19		Aqueous Solubility Prediction Method
logp	0.727		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1586.10		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	666.20	K	Joback Method
tc	852.42	K	Joback Method
tf	370.27	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.34	J/mol×K	666.20	Joback Method
cpg	396.62	J/mol×K	697.24	Joback Method
cpg	406.35	J/mol×K	728.27	Joback Method
cpg	415.54	J/mol×K	759.31	Joback Method
cpg	424.21	J/mol×K	790.35	Joback Method
cpg	432.37	J/mol×K	821.39	Joback Method
cpg	440.03	J/mol×K	852.42	Joback Method
dvisc	0.0047133	Pa×s	370.27	Joback Method
dvisc	0.0010161	Pa×s	419.59	Joback Method
dvisc	0.0003025	Pa×s	468.91	Joback Method
dvisc	0.0001134	Pa×s	518.24	Joback Method
dvisc	0.0000504	Pa×s	567.56	Joback Method
dvisc	0.0000255	Pa×s	616.88	Joback Method
dvisc	0.0000143	Pa×s	666.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.70	K	0.50	NIST Webbook

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=C59472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Study of Glass Transition Phenomena in the Supercooled Liquid Phase of Methocarbamol, Acetaminophen and Mephensin:	https://www.doi.org/10.1016/j.tca.2013.10.035

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume