Methocarbamol

Other names:

1,2-Propanediol, 3-(2-methoxyphenoxy)-, 1-carbamate
1,2-Propanediol, 3-(o-methoxyphenoxy)-, 1-carbamate
2-Hydroxy-3-(o-methoxyphenoxy)propyl 1-carbamate
2-Hydroxy-3-(o-methoxyphenoxy)propyl carbamate
2-hydroxy-3-(2-methoxyphenoxy)propyl carbamate
3-(2-Methoxyphenoxy)-1-glyceryl carbamate
3-(o-Methoxyphenoxy)-1,2-propanediol 1-carbamate
3-(o-Methoxyphenoxy)-2-hydroxypropyl carbamate
3-O-(2-Methoxyphenyl)-1-glyceryl carbamate
AHR 85
Avetil
Carbamic acid, 2-hydroxy-3-(o-methoxyphenoxy)propyl ester
Delaxin
Etroflex
Glycerylguaiacolate Carbamate
Glycerylguajacol-Carbamat
Guaiacol glyceryl ether carbamate
Guaiphenesin carbamate
Guaiphenesine carbamate
Guiacol-gliceriletere monocarbammato
Lumirelax
Methocal
Metocarbamol
Metocarbamolo
Metofenia
Metofenina
Miolaxene
Miorilas
Miowas
Myolaxene
NSC 170960
Neuraxin
Parabaxin
Perilax
Reflexyn
Relax
Relestrid
Robamol
Robaxan
Robaxin

	Robaxine
	Robaxon
	Robinax
	Romethocarb
	Surquetil
	Traumacut
	Tresortil
Inchi:	InChI=1S/C11H15NO5/c1-15-9-4-2-3-5-10(9)16-6-8(13)7-17-11(12)14/h2-5,8,13H,6-7H2
InchiKey:	GNXFOGHNGIVQEH-UHFFFAOYSA-N
Formula:	C11H15NO5
SMILES:	COc1ccccc1OCC(O)COC(=N)O
Mol. weight [g/mol]:	241.24
CAS:	532-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-242.96	kJ/mol	Joback Method
hf	-553.38	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Study of Glass Transition Phenomena in the Supercooled Liquid Phase of Methocarbamol, Acetaminophen and Mephensin
hvap	95.30	kJ/mol	Joback Method
log10ws	-1.13		Aqueous Solubility Prediction Method
log10ws	-0.98		Estimated Solubility Method
logp	0.944		Crippen Method
mcvol	177.120	ml/mol	McGowan Method
tb	818.26	K	Joback Method
tf	494.78	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.31	J/mol×K	818.26	Joback Method
cpg	123.73	J/mol×K	100.12	Joback Method

cpg	123.73	J/mol×K	100.12	Joback Method
cpg	123.73	J/mol×K	100.12	Joback Method
cpg	123.73	J/mol×K	100.12	Joback Method
cpg	123.73	J/mol×K	100.12	Joback Method
cpg	123.73	J/mol×K	100.12	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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C532036&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point