Metoclopramide

Other names:	2-Methoxy-4-amino-5-chloro-N,N-dimethylaminoethylbenzamide
	2-Methoxy-5-Chloroprocainamide
	4-Amino-5-chloro-2-methoxy-N-(«beta»-diethylaminoethyl)benzamide
	4-Amino-5-chloro-2-methoxy-N-(Â«betaÂ»-diethylaminoethyl)benzamide
	4-Amino-5-chloro-N-(2-(diethylamino)ethyl)-2-methoxybenzamide
	5-Chloro-2-methoxyprocainamide
	Benzamide, 4-amino-5-chloro-N-[2-(diethylamino)ethyl]-2-methoxy-
	DEL 1267
	Gastromax
	Maxeran
	Metaclopramide
	Metaclopromide
	Methochlopramide
	Methoclopramide
	Metochlopramide
	Metoclol
	Metocobil
	Metramid
	Moriperan
	N-(Diethylaminoethyl)-2-methoxy-4-amino-5-chlorobenzamide
	Parmid
	Plasil
	Plasil (pharmaceutical)
	Primperan
	Regla
	Reliveran
	o-Anisamide, 4-amino-5-chloro-N-[2-(diethylamino)ethyl]-
Inchi:	InChI=1S/C14H22ClN3O2/c1-4-18(5-2)7-6-17-14(19)10-8-11(15)12(16)9-13(10)20-3/h8-9
InchiKey:	TTWJBBZEZQICBI-UHFFFAOYSA-N
Formula:	C14H22ClN3O2
SMILES:	CCN(CC)CCNC(=O)c1cc(Cl)c(N)cc1OC
Mol. weight [g/mol]:	299.80
CAS:	364-62-5

Physical Properties

Property code	Value	Unit	Source

gf	171.29	kJ/mol	Joback Method
hf	-235.92	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	83.68	kJ/mol	Joback Method
log10ws	-3.57		Aqueous Solubility Prediction Method
logp	2.002		Crippen Method
mcvol	233.980	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2624.00		NIST Webbook
rinpol	2602.00		NIST Webbook
rinpol	2630.00		NIST Webbook
rinpol	2602.00		NIST Webbook
rinpol	2630.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	810.20	K	Joback Method
tc	1021.97	K	Joback Method
tf	581.99	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.85	J/mol×K	810.20	Joback Method
cpg	692.36	J/mol×K	845.50	Joback Method
cpg	704.91	J/mol×K	880.79	Joback Method
cpg	716.54	J/mol×K	916.09	Joback Method
cpg	727.27	J/mol×K	951.38	Joback Method
cpg	737.13	J/mol×K	986.68	Joback Method
cpg	746.15	J/mol×K	1021.97	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C364625&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume