

Bromopride

Other names:

Benzamide, 4-amino-5-bromo-N-[2-(diethylamino)ethyl]-2-methoxy-
o-Anisamide, 4-amino-5-bromo-N-[2-(diethylamino)ethyl]-
4-Amino-5-bromo-N-(2-(diethylamino)ethyl)-o-anisamide
Artomey
Bromoprida
VAL 13081
Valopride
Emepride
Emoril
Viadil

Inchi:

InChI=1S/C14H22BrN3O2/c1-4-18(5-2)7-6-17-14(19)10-8-11(15)12(16)9-13(10)20-3/h8-

InchiKey:

GIYAQDDTCWHPPL-UHFFFAOYSA-N

Formula:

C14H22BrN3O2

SMILES:

CCN(CC)CCNC(=O)c1cc(Br)c(N)cc1OC

Mol. weight [g/mol]:

344.25

CAS:

4093-35-0

Physical Properties

Property code	Value	Unit	Source
gf	197.54	kJ/mol	Joback Method
hf	-193.85	kJ/mol	Joback Method
hfus	46.28	kJ/mol	Joback Method
hvap	85.73	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.112		Crippen Method
mcvol	239.240	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	2742.00		NIST Webbook
tb	838.93	K	Joback Method
tc	1057.06	K	Joback Method
tf	611.87	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.48	J/mol×K	838.93	Joback Method
cpg	703.56	J/mol×K	875.29	Joback Method
cpg	715.68	J/mol×K	911.64	Joback Method
cpg	726.90	J/mol×K	948.00	Joback Method
cpg	737.24	J/mol×K	984.35	Joback Method
cpg	746.75	J/mol×K	1020.71	Joback Method
cpg	755.47	J/mol×K	1057.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4093350&Units=SI

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

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