Chlorbufam

Other names:	Carbamic acid, (3-chlorophenyl)-, 1-methyl-2-propynyl ester
	Carbanilic acid, m-chloro-, 1-methyl-2-propynyl ester
	BIPC
	Chlorbupham
	Chlorobufam
	Grisemin
	1-Butyn-3-yl m-chlorophenylcarbamate
	BICP
	3-Butyn-2-ol, m-chlorocarbanilate
	Butyn-1-ol-3-ester of m-chlorophenylcarbamic acid
	3-Butynyl-m-chlorocarbanilate
	Chlorbufame
	3-Chlorophenylcarbamic acid 1-methylpropynyl ester
	3-Chlorphenyl-carbamidsaure-butin-(1)-yl(3)-ester
	Grisin
	IEM-1-15
	Isobutinyl-N-(3-chlorphenyl)-carbamat
	1-Methyl-2-propynyl m-chlorocarbanilate
	1-Methyl-2-propynyl m-chlorophenylcarbamate
	1-Methylpropynyl 3-chlorophenylcarbamate
	1-Methylpropynyl ester of 3-chlorophenylcarbamic acid
Inchi:	InChI=1S/C11H10ClNO2/c1-3-8(2)15-11(14)13-10-6-4-5-9(12)7-10/h1,4-8H,2H3,(H,13,1
InchiKey:	ULBXWWGWDPVHAO-UHFFFAOYSA-N
Formula:	C11H10ClNO2
SMILES:	C#CC(C)OC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]:	223.66
CAS:	1967-16-4

Physical Properties

Property code	Value	Unit	Source
gf	208.69	kJ/mol	Joback Method
hf	34.24	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.910		Crippen Method

mcvol	163.150	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	636.31	K	Joback Method
tc	869.20	K	Joback Method
tf	439.38	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.99	J/mol×K	636.31	Joback Method
cpg	391.00	J/mol×K	675.12	Joback Method
cpg	402.15	J/mol×K	713.94	Joback Method
cpg	412.46	J/mol×K	752.75	Joback Method
cpg	421.98	J/mol×K	791.57	Joback Method
cpg	430.73	J/mol×K	830.38	Joback Method
cpg	438.75	J/mol×K	869.20	Joback Method

Sources

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=C1967164&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume