Carbamic acid, (3-chlorophenyl)-, 1-methyl-2-propynyl ester

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

Physical Properties

Property code	Value	Unit	Source
hfus	29.43	kJ/mol	Joback Method
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	2.910		Crippen Method
mcvol	163.150	ml/mol	McGowan Method
tb	555.13	K	Cheméo Relay (1.0)
tf	327.84	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1967164&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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