Carbamic acid, (3-chlorophenyl)-, 1-methylethyl ester

Other names:

(3-Chlorophenyl)carbamic acid, 1-methylethyl ester
3-Chlorocarbanilic acid, isopropyl ester
Beet-Kleen
Bygran
CI-IPC
CIPC
Carbamic acid, N-(3-chlorophenyl)-, 1-methylethyl ester
Carbanilic acid, m-chloro-, isopropyl ester
Chlor IFC
Chlor IFK
ChlorIPC
Chloro-IFK
Chloro-IPC
Chloropham
Chloropropham
Chlorprophame
Cl-IFK
ENT 18,060
Elbanil
Fasco WY-HOE
Furloe
Furloe 3 EC
Isopropyl 3-chlorocarbanilate
Isopropyl 3-chlorophenylcarbamate
Isopropyl N-(3-chlorophenyl)carbamate
Isopropyl N-(m-chlorophenyl)carbamate
Isopropyl N-chlorophenylcarbamate
Isopropyl chlorocarbanilate
Isopropyl m-chlorocarbanilate
Jack Wilson chloro 51(oil)
Keim-Stop
Liro CIPC
Metoxon
Mirvale
N-(3-Chloor-fenyl)-isopropyl carbamaat
N-(3-Chlor-phenyl)-isopropyl-carbamat
N-(3-Chloro phenyl)carbamate d'isopropyle
N-(3-Chlorophenyl)carbamic acid, isopropyl ester
N-(3-Chlorophenyl)isopropyl carbamate
N-(3-Cloro-fenil)-isopropil-carbammato

	Nexoval
	Prevenol 56
	Preventol
	Preventol 56
	Preweed
	Sprout Nip
	Spud-Nic
	Spud-Nie
	Stopgerme-S
	Taterpex
	Triherbicide CIPC
	Y 3
	m-Chlorocarbanilic acid isopropyl ester
	propan-2-yl N-(3-chlorophenyl)carbamate
Inchi:	InChI=1S/C10H12ClNO2/c1-7(2)14-10(13)12-9-5-3-4-8(11)6-9/h3-7H,1-2H3,(H,12,13)
InchiKey:	CWJSHJJYOPWUGX-UHFFFAOYSA-N
Formula:	C10H12ClNO2
SMILES:	CC(C)OC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]:	213.66

Physical Properties

Property code	Value	Unit	Source
hfus	23.87	kJ/mol	Joback Method
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-3.38		Estimated Solubility Method
log10ws	-3.38		Aqueous Solubility Prediction Method
logp	3.297		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook

rinpol	1626.00		NIST Webbook
rinpol	1613.00		NIST Webbook
ripol	2643.00		NIST Webbook
tb	536.49	K	Cheméo Relay (1.0)
tf	315.00 ± 0.20	K	NIST Webbook
tf	315.70 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.44	J/mol×K	623.31	Joback Method
cpg	386.15	J/mol×K	660.30	Joback Method
cpg	398.05	J/mol×K	697.28	Joback Method
cpg	409.13	J/mol×K	734.27	Joback Method
cpg	419.44	J/mol×K	771.25	Joback Method
cpg	428.97	J/mol×K	808.24	Joback Method
cpg	437.76	J/mol×K	845.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	0.30	NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101213&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point