Barban

Other names:	(3-Chlorophenyl)carbamic acid 4-chloro-2-butynyl ester
	(4-Chloor-but-2-yn-yl)-N-(3-chloor-fenyl)-carbamaat
	(4-Chlor-but-2-in-yl)-N-(3-chlor-phenyl)-carbamat
	(4-Cloro-but-2-in-il)-N-(3-cloro-fenil)-carbammato
	2-Butyn-1-ol, 4-chloro-, m-chlorocarbanilate
	2-Butynyl 4-chloro-m-chlorocarbanilate
	4-Chloro-2-Butynyl m-chlorocarbanilate
	4-Chloro-2-butynyl 3-chlorocarbanilate
	4-Chloro-2-butynyl N-(3-chlorophenyl)carbamate
	4-Chlorobut-2-ynyl 3-chlorophenylcarbamate
	4-Chlorobut-2-ynyl-m-chlorocarbanilate
	4-chlorobut-2-ynyl N-(3-chlorophenyl)carbamate
	A 980
	Barbamate
	Barbanate
	Barbane
	C-847
	CBN
	CS-847
	Carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester
	Carbanilic acid, m-chloro-, 4-chloro-2-butynyl ester
	Carbin
	Carbine
	Carbyne
	Carbyne (Herbicide)
	Caryne
	Chlorinat
	Chloro-2-butynyl m-chlorocarbamate
	Fisons B25
	Karbin
	N-(3-Chloro phenyl)carbamate de 4-chloro 2-butynyle
	NSC 29168
	Neoban
	S 847
	m-Chlorocarbanilic acid, 4-chloro-2-butynyl ester
Inchi:	InChI=1S/C11H9Cl2NO2/c12-6-1-2-7-16-11(15)14-10-5-3-4-9(13)8-10/h3-5,8H,6-7H2,(H
InchiKey:	MCOQHIWZJUDQIC-UHFFFAOYSA-N
Formula:	C11H9Cl2NO2
SMILES:	O=C(Nc1cccc(Cl)c1)OCC#CCCl
Mol. weight [g/mol]:	258.10

CAS: 101-27-9

Physical Properties

Property code	Value	Unit	Source
gf	178.93	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-4.37		Estimated Solubility Method
log10ws	-4.37		Aqueous Solubility Prediction Method
logp	3.131		Crippen Method
mcvol	175.390	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	693.06	K	Joback Method
tc	934.38	K	Joback Method
tf	345.59 ± 0.20	K	NIST Webbook
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.56	J/mol×K	693.06	Joback Method
cpg	411.71	J/mol×K	733.28	Joback Method
cpg	422.00	J/mol×K	773.50	Joback Method
cpg	431.46	J/mol×K	813.72	Joback Method
cpg	440.11	J/mol×K	853.94	Joback Method
cpg	447.97	J/mol×K	894.16	Joback Method
cpg	455.07	J/mol×K	934.38	Joback Method
hfust	26.91	kJ/mol	344.10	NIST Webbook
hfust	26.91	kJ/mol	344.10	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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