Benthiocarb

Other names:	B 3015
	Bolero
	Carbamic acid, diethylthio-, S-(p-chlorobenzyl) ester
	Carbamothioic acid, diethyl-, S-[(4-chlorophenyl)methyl] ester
	IMC 3950
	S-((4-Chlorophenyl)methyl)diethylcarbamothioate
	S-(4-Chlorobenzyl) N,N-diethylthiocarbamate
	S-(4-Chlorobenzyl) diethylthiocarbamate
	S-(4-Chlorobenzyl) diethylthiolcarbamate
	S-(p-Chlorobenzyl) diethylthiocarbamate
	S-[(4-chlorophenyl)methyl] diethylaminomethanethioate
	Saturn
	Saturn (pesticide)
	Saturno
	Siacarb
	Thiobencarb
	Thiobencarbe
	p-Chlorobenzyl N,N-diethylthiolcarbamate
	p-Chlorobenzyl diethylthiolcarbamate
Inchi:	InChI=1S/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-5-7-11(13)8-6-10/h5-8H,3-4,9H2,1-
InchiKey:	QHTQREMOGMZHJV-UHFFFAOYSA-N
Formula:	C12H16ClNOS
SMILES:	CCN(CC)C(=O)SCc1ccc(Cl)cc1
Mol. weight [g/mol]:	257.78
CAS:	28249-77-6

Physical Properties

Property code	Value	Unit	Source
gf	155.99	kJ/mol	Joback Method
hf	-84.87	kJ/mol	Joback Method
hfus	33.43	kJ/mol	Joback Method
hvap	65.23	kJ/mol	Joback Method
log10ws	-3.93		Aqueous Solubility Prediction Method
logp	4.035		Crippen Method
mcvol	196.320	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method

rinpol	1985.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	678.14	K	Joback Method
tc	904.46	K	Joback Method
tf	276.45	K	Aqueous Solubility Prediction Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.62	J/mol×K	678.14	Joback Method
cpg	500.93	J/mol×K	715.86	Joback Method
cpg	514.20	J/mol×K	753.58	Joback Method
cpg	526.49	J/mol×K	791.30	Joback Method
cpg	537.84	J/mol×K	829.02	Joback Method
cpg	548.30	J/mol×K	866.74	Joback Method
cpg	557.91	J/mol×K	904.46	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28249776&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
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