Propachlor

Other names:	2-Chloro-N-(1-methylethyl)-N-phenylacetamide
	2-Chloro-N-isopropyl-N-phenylacetamide
	2-Chloro-N-isopropylacetanilide
	2-chloro-N-phenyl-N-propan-2-ylacetamide
	Acetamide, 2-chloro-N-(1-methylethyl)-N-phenyl-
	Acetanilide, 2-chloro-N-isopropyl-
	Acilid
	Albrass
	Bexton
	Bexton 4L
	CP 31393
	Chloressigsaeure-N-isopropylanilid
	Kartex A
	Muharicid
	N-Isopropyl-2-chloroacetanilide
	N-Isopropyl-«alpha»-Chloroacetanilide
	N-Isopropyl-Â«alphaÂ»-Chloroacetanilide
	Nitacid
	Niticid
	Prolex
	Propachlore
	Ramrod
	Ramrod 20G
	Ramrod 65
	Satecid
	Tripart sentinel
	«alpha»-Chloro-N-isopropylacetanilide
	Â«alphaÂ»-Chloro-N-isopropylacetanilide
Inchi:	InChI=1S/C11H14ClNO/c1-9(2)13(11(14)8-12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	MFOUDYKPLGXPGO-UHFFFAOYSA-N
Formula:	C11H14ClNO
SMILES:	CC(C)N(C(=O)CCl)c1ccccc1
Mol. weight [g/mol]:	211.69
CAS:	1918-16-7

Physical Properties

Property code	Value	Unit	Source

gf	121.64	kJ/mol	Joback Method
hf	-99.91	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-2.48		Aqueous Solubility Prediction Method
log10ws	-2.48		Estimated Solubility Method
logp	2.667		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1612.00		NIST Webbook
ripol	2345.00		NIST Webbook
tb	581.06	K	Joback Method
tc	798.35	K	Joback Method
tf	337.47	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.07	J/mol×K	581.06	Joback Method
cpg	399.84	J/mol×K	617.28	Joback Method
cpg	413.60	J/mol×K	653.49	Joback Method
cpg	426.40	J/mol×K	689.71	Joback Method
cpg	438.29	J/mol×K	725.92	Joback Method
cpg	449.32	J/mol×K	762.14	Joback Method
cpg	459.55	J/mol×K	798.35	Joback Method

Sources

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=C1918167&Units=SI

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

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

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

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