Propanil

Other names:

3',4'-Dichloropropioanilide
3',4'-Dichloropropionanilide
BAY 30130
Cekupropanil
Chem Rice
DCPA
DPA
Dichloropropionanilide
Dipram
Erbanil
FW 734
Grascide
Herbax
Montrose propanil
N-(3,4-Dichlorophenyl)propanamide
N-(3,4-Dichlorophenyl)propionamide
NSC 31312
Prop job
Propanamide, N-(3,4-dichlorophenyl)-
Propanex
Propanid
Propanide
Propanile
Propionanilide, 3',4'-dichloro-
Propionic acid 3,4-dichloroanilide
Riselect
Rogue
S 10165
Stam
Stam 80EDF
Stam F 34
Stam LV 10
Stam M-4
Stampede
Stampede 360
Strel
Supernox
Surcopur
Surpur
Synpran N

	Wham EZ
Inchi:	InChI=1S/C9H9Cl2NO/c1-2-9(13)12-6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3,(H,12,13)
InchiKey:	LFULEKSKNZEWOE-UHFFFAOYSA-N
Formula:	C9H9Cl2NO
SMILES:	CCC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	218.08
CAS:	709-98-8

Physical Properties

Property code	Value	Unit	Source
gf	54.66	kJ/mol	Joback Method
hf	-106.09	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-2.88		Aqueous Solubility Prediction Method
log10ws	-3.00		Estimated Solubility Method
logp	3.342		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1879.00		NIST Webbook
ripol	3197.00		NIST Webbook
ripol	3197.00		NIST Webbook
tb	620.86	K	Joback Method
tc	849.72	K	Joback Method
tf	364.30 ± 0.20	K	NIST Webbook
tf	364.50 ± 0.20	K	NIST Webbook
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.69	J/mol×K	620.86	Joback Method
cpg	335.35	J/mol×K	659.00	Joback Method
cpg	345.28	J/mol×K	697.15	Joback Method
cpg	354.50	J/mol×K	735.29	Joback Method
cpg	363.05	J/mol×K	773.43	Joback Method
cpg	370.94	J/mol×K	811.58	Joback Method
cpg	378.22	J/mol×K	849.72	Joback Method
hfust	18.26	kJ/mol	363.70	NIST Webbook

Sources

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
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=C709988&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume