Alachlor

Other names: 2-Chloro-2',6'-diethyl-N-(methoxymethyl)acetanilide
2-Chloro-N-(2,6-diethyl)phenyl-N-methoxymethylacetamide
2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide
2-chloro-N-(methoxymethyl)-N-(2,6-diethyl-phenyl)-acetamide
Acetamide, 2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)-
Acetanilide, 2-chloro-2',6'-diethyl-N-(methoxymethyl)-
Alachlore
Alanex
Alanox
Alatox 480
Alazine
Alochlor
CP 50144
Chloressigsaeure-N-(methoxymethyl)-2,6-diaethylanilid
Lasagrin
Lasso
Lasso micro-tech
Lazo
Metachlor
Methachlor
Pillarzo
alachlor [2-chloro-N-(methoxymethyl)-N-(2',6'-diethyl-phenyl)-acetamide]

Inchi: InChI=1S/C14H20ClNO2/c1-4-11-7-6-8-12(5-2)14(11)16(10-18-3)13(17)9-15/h6-8H,4-5,9

InchiKey: XCSGPAVHZFQHGE-UHFFFAOYSA-N

Formula: C14H20ClNO2

SMILES: CCc1cccc(CC)c1N(COC)C(=O)CCl

Mol. weight [g/mol]: 269.77

CAS: 15972-60-8

Physical Properties

Property code	Value	Unit	Source
gf	25.08	kJ/mol	Joback Method
hf	-311.71	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	65.94	kJ/mol	Joback Method
log10ws	-3.26		Estimated Solubility Method

log10ws	-3.15		Aqueous Solubility Prediction Method
logp	2.987		Crippen Method
mcvol	214.020	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1882.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1899.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	320.08		NIST Webbook
rinpol	1896.00		NIST Webbook
rinpol	320.08		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	682.52	K	Joback Method
tc	885.67	K	Joback Method
tf	316.71 ± 0.20	K	NIST Webbook
tf	315.00 ± 0.20	K	NIST Webbook
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.02	J/mol×K	682.52	Joback Method
cpg	576.24	J/mol×K	716.38	Joback Method
cpg	590.56	J/mol×K	750.24	Joback Method
cpg	604.00	J/mol×K	784.10	Joback Method
cpg	616.59	J/mol×K	817.95	Joback Method
cpg	628.35	J/mol×K	851.81	Joback Method
cpg	639.32	J/mol×K	885.67	Joback Method
hfust	26.70	kJ/mol	317.70	NIST Webbook
hfust	25.31	kJ/mol	315.90	NIST Webbook
hvapt	85.00 ± 1.00	kJ/mol	436.00	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=C15972608&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
hvapt:	Enthalpy of vaporization at a given temperature
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