Metolachlor

Other names:	2-Chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide
	2-chloro-2'-ethyl-N-(2-methoxy-1-methylethyl)-6'-methylacetanilide
	2-chloro-N-(2-ethyl-6-methylphenyl)-N-(1-methoxypropan-2-yl)acetamide
	Acetamide, 2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)-
	CGA 24705
	Codal
	Dual
	Dual 720EC
	Dual 8E
	Dual 960 EC
	Dual II
	Dual Magnum
	Dual Triple
	Metetilachlor
	N-(1-Methyl-2-methoxyethyl)-N-chloroacetyl-2-ethyl-6-methylaniline
	Ontrack 8E
	Pennant
	Yibingjiacaoan
Inchi:	InChI=1S/C15H22ClNO2/c1-5-13-8-6-7-11(2)15(13)17(14(18)9-16)12(3)10-19-4/h6-8,12I
InchiKey:	WVQBLGZPHOPPFO-UHFFFAOYSA-N
Formula:	C15H22ClNO2
SMILES:	CCc1cccc(C)c1N(C(=O)CCl)C(C)COC
Mol. weight [g/mol]:	283.79
CAS:	51218-45-2

Physical Properties

Property code	Value	Unit	Source
gf	31.06	kJ/mol	Joback Method
hf	-337.63	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	67.78	kJ/mol	Joback Method
log10ws	-2.73		Estimated Solubility Method
log10ws	-2.73		Aqueous Solubility Prediction Method
logp	3.164		Crippen Method
mcvol	228.110	ml/mol	McGowan Method

pc	1823.17	kPa	Joback Method
tb	704.96	K	Joback Method
tc	909.07	K	Joback Method
tf	247.45	K	Aqueous Solubility Prediction Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.02	J/mol×K	841.03	Joback Method
cpg	685.22	J/mol×K	875.05	Joback Method
cpg	615.13	J/mol×K	704.96	Joback Method
cpg	631.03	J/mol×K	738.98	Joback Method
cpg	645.95	J/mol×K	773.00	Joback Method
cpg	659.94	J/mol×K	807.01	Joback Method
cpg	696.56	J/mol×K	909.07	Joback Method
hfust	17.00	kJ/mol	299.00	NIST Webbook
hvapt	70.00 ± 1.00	kJ/mol	436.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51218452&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
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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