Metalaxyl

Other names:	(.+/-.)-Metalaxyl
	Alanine, N-(2,6-dimethylphenyl)-N-(methoxyacetyl)-, methyl ester
	Alanine, N-(methoxyacetyl)-N-(2,6-xylyl)-, methyl ester, DL-
	Allegiance
	Apron
	Apron FL
	Apron SD 35
	CG 117
	CGA-48988
	DL-Alanine, N-(2,6-dimethylphenyl)-N-(methoxyacetyl)-, methyl ester
	IPO-FS
	Jiashuangling
	Metalasyl
	Metalaxil
	Metanaxin
	Metasyl
	Metaxanin
	Methyl N-(2,6-dimethylphenyl)-N-(methoxyacetyl)-DL-alaninate
	Methyl N-(2-methoxyacetyl)-n-(2,6-xylyl)-(dl)-alaninate
	N-(2,6-Dimethylphenyl)-N-(methoxyacetyl)-dl-alanine methyl ester
	Ridomil
	Ridomil 72WP
	Ridomil Vino
	Subdue
Inchi:	InChI=1S/C15H21NO4/c1-10-7-6-8-11(2)14(10)16(13(17)9-19-4)12(3)15(18)20-5/h6-8,12
InchiKey:	ZQEIXNIJLIKNTD-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	COCC(=O)N(c1c(C)cccc1C)C(C)C(=O)OC
Mol. weight [g/mol]:	279.33
CAS:	57837-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-190.93	kJ/mol	Joback Method
hf	-566.69	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method

hvap	72.55	kJ/mol	Joback Method
log10ws	-1.60		Aqueous Solubility Prediction Method
log10ws	-1.60		Estimated Solubility Method
logp	1.844		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	743.82	K	Joback Method
tc	949.44	K	Joback Method
tf	346.17 ± 0.20	K	NIST Webbook
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.69	J/mol×K	915.17	Joback Method
cpg	633.37	J/mol×K	743.82	Joback Method
cpg	648.40	J/mol×K	778.09	Joback Method
cpg	662.44	J/mol×K	812.36	Joback Method
cpg	675.49	J/mol×K	846.63	Joback Method
cpg	687.57	J/mol×K	880.90	Joback Method
cpg	708.87	J/mol×K	949.44	Joback Method
hfust	26.46	kJ/mol	345.50	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=C57837191&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume