Aminocarb

Other names:	(4-Dimethylamino-3-methyl-phenyl)N-methyl-carbamaat
	(4-Dimethylamino-3-methyl-phenyl)N-methyl-carbamat
	(4-Dimethylamino-3-methyl-phenyl)N-methyl-carbamate
	(4-Dimetilamino-3-metil-fenil)-N-metil-carbammato
	3-Methyl-4-(Dimethylamino)phenyl methylcarbamate
	4-(Dimethylamino)-3-cresyl methylcarbamate
	4-(Dimethylamino)-3-methylphenol methyl carbamate
	4-(Dimethylamino)-3-tolyl methylcarbamate
	4-(Dimethylamino)-m-tolyl methylcarbamate
	4-Dimethylamino- m-cresyl methylcarbamate
	4-Dimethylamino-3-methylphenyl methylcarbamate
	A 363
	Aminocarbe
	BAY 44646
	BAYER 44646
	Bayer 5080
	Carbamic acid, methyl-, 4-(dimethylamino)-3-methylphenyl ester
	Carbamic acid, methyl-, 4-(dimethylamino)-m-tolyl ester
	ENT 25,784
	Matacil
	Matacil 180D
	Mitacil
	N-Methylcarbamate de 4-dimethylamino 3-methyl phenyle
	Phenol, 4-(dimethylamino)-3-methyl-, methylcarbamate
	Phenol, 4-(dimethylamino)-3-methyl-, methylcarbamate (ester)
	m-Cresol, 4-(dimethylamino)-, methylcarbamate
Inchi:	InChI=1S/C11H16N2O2/c1-8-7-9(15-11(14)12-2)5-6-10(8)13(3)4/h5-7H,1-4H3,(H,12,14)
InchiKey:	IMIDOCRTMDIQIJ-UHFFFAOYSA-N
Formula:	C11H16N2O2
SMILES:	CNC(=O)Oc1ccc(N(C)C)c(C)c1
Mol. weight [g/mol]:	208.26
CAS:	2032-59-9

Physical Properties

Property code	Value	Unit	Source
gf	101.14	kJ/mol	Joback Method

hf	-180.58	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	61.31	kJ/mol	Joback Method
log10ws	-2.36		Aqueous Solubility Prediction Method
log10ws	-2.36		Estimated Solubility Method
logp	1.779		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	626.62	K	Joback Method
tc	834.88	K	Joback Method
tf	368.00 ± 0.20	K	NIST Webbook
tf	366.65	K	Aqueous Solubility Prediction Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.98	J/mol×K	626.62	Joback Method
cpg	446.23	J/mol×K	661.33	Joback Method
cpg	459.65	J/mol×K	696.04	Joback Method
cpg	472.26	J/mol×K	730.75	Joback Method
cpg	484.08	J/mol×K	765.46	Joback Method
cpg	495.12	J/mol×K	800.17	Joback Method
cpg	505.41	J/mol×K	834.88	Joback Method

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=C2032599&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
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