Phenol, 3,5-dimethyl-, methylcarbamate

Other names:	3,5-Dimethylphenyl N-methylcarbamate
	3,5-Dimethylphenyl methylcarbamate
	3,5-Xmc
	3,5-Xylenol, methylcarbamate
	3,5-Xylenyl N-methylcarbamate
	3,5-Xylyl N-methylcarbamate
	3,5-Xylyl methylcarbamate
	3,5-Xylylester kyseliny methylkarbaminove
	Carbamic acid, methyl-, 3,5-xylyl ester
	Cosban
	DRC 3340
	H-69
	Macbal
	Maqbarl
	Methylcarbamic acid 3,5-xylyl ester
	NSC 35375
	Phenol, 3,5-dimethyl-, 1-(N-methylcarbamate)
	S 1041
	XMC
	XMC (Pesticide)
Inchi:	InChI=1S/C10H13NO2/c1-7-4-8(2)6-9(5-7)13-10(12)11-3/h4-6H,1-3H3,(H,11,12)
InchiKey:	CVQODEWAPZVVBU-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CNC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	179.22
CAS:	2655-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-18.06	kJ/mol	Joback Method
hf	-227.47	kJ/mol	Joback Method
hfus	22.81	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-2.58		Aqueous Solubility Prediction Method
log10ws	-2.58		Estimated Solubility Method

logp	2.022		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
ripol	2173.00		NIST Webbook
tb	591.30	K	Joback Method
tc	805.99	K	Joback Method
tf	378.74	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.95	J/mol×K	591.30	Joback Method
cpg	360.01	J/mol×K	627.08	Joback Method
cpg	372.35	J/mol×K	662.86	Joback Method
cpg	383.98	J/mol×K	698.65	Joback Method
cpg	394.92	J/mol×K	734.43	Joback Method
cpg	405.16	J/mol×K	770.21	Joback Method
cpg	414.72	J/mol×K	805.99	Joback Method

Sources

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=C2655143&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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