Methiocarb

Other names:	(3,5-dimethyl-4-methylsulfanylphenyl) N-methylcarbamate
	3,5-Dimethyl-4-(Methylthio)phenyl methylcarbamate
	3,5-Dimethyl-4-(methylthio)phenol methylcarbamate
	3,5-Dimethyl-4-methyl-thiophenyl-N-carbamat
	3,5-Dimethyl-4-methylthiophenyl N-methylcarbamate
	3,5-Xylenol, 4-(methylthio)-, methylcarbamate
	4-(Methylthio)-3,5-dimethylphenyl methylcarbamate
	4-(Methylthio)-3,5-xylyl methylcarbamate
	4-Methylmercapto-3,5-dimethylphenyl N-methylcarbamate
	4-Methylmercapto-3,5-xylyl methylcarbamate
	B 37344
	BAY 37344
	BAY 5024
	BAY 9026
	BAYER 37344
	Carbamic acid, 3,5-dimethyl-4-methylthiophenyl ester, N-methyl
	Carbamic acid, N-methyl-, 4-(methylthio)-3,5-xylyl ester
	Carbamic acid, methyl-, 3,5-dimethyl-4-(methylthio)phenyl ester
	Carbamic acid, methyl-, 4-(methylthio)-3,5-xylyl ester
	Club
	DCR 736
	Draza
	ENT 25,726
	H 321
	Mercaptodimethur
	Mesurol
	Mesurol phenol
	Methiocarbe
	Methyl carbamic acid 4-(methylthio)-3,5-xylyl ester
	Metmercapturan
	Metmercapturon
	OMS-93
	Phenol, 3,5-dimethyl-4-(methylthio)-, methylcarbamate
	Phenyl-3,5-dimethyl-4-(methylthio)-, methylcarbamate
	SD 9228
Inchi:	InChI=1S/C11H15NO2S/c1-7-5-9(14-11(13)12-3)6-8(2)10(7)15-4/h5-6H,1-4H3,(H,12,13)
InchiKey:	YFBPRJGDJKVWAH-UHFFFAOYSA-N
Formula:	C11H15NO2S
SMILES:	CNC(=O)Oc1cc(C)c(SC)c(C)c1
Mol. weight [g/mol]:	225.31

CAS: 2032-65-7

Physical Properties

Property code	Value	Unit	Source
gf	13.85	kJ/mol	Joback Method
hf	-217.71	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-3.92		Aqueous Solubility Prediction Method
logp	2.744		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1956.00		NIST Webbook
tb	687.94	K	Joback Method
tc	915.89	K	Joback Method
tf	394.80 ± 0.20	K	NIST Webbook
tf	394.44 ± 0.20	K	NIST Webbook
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.93	J/mol×K	687.94	Joback Method
cpg	459.40	J/mol×K	725.93	Joback Method
cpg	471.99	J/mol×K	763.92	Joback Method
cpg	483.69	J/mol×K	801.91	Joback Method
cpg	494.49	J/mol×K	839.91	Joback Method
cpg	504.41	J/mol×K	877.90	Joback Method
cpg	513.43	J/mol×K	915.89	Joback Method
hfust	30.36	kJ/mol	393.80	NIST Webbook
hfust	30.36	kJ/mol	393.80	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2032657&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