Pyrolan

Other names:	1-Fenyl-3-methyl-5-pyrazolylester kyseliny dimethylkarbaminove
	1-Phenyl-3-methyl-5-pyrazolyl N,N-dimethyl carbamate
	3-Methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate
	3-Methyl-1-phenyl-5-pyrazolyl dimethyl carbamate
	3-Methyl-1-phenylpyrazol-5-yl dimethyl carbamate
	Carbamic acid, dimethyl-, 3-methyl-1-phenyl-1H-pyrazol-5-yl ester
	Carbamic acid, dimethyl-, 3-methyl-1-phenylpyrazol-5-yl ester
	Carbamic acid, dimethyl-, 5-methyl-2-phenyl-pyrazol-3-yl ester
	Dimethyl 5-(3-methyl-1-phenylpyrazolyl) carbamate
	Dimethylcarbamic acid 3-methyl-1-phenyl-1H-pyrazol-5-yl ester
	Dimethylcarbamic acid, 3-methyl-1-phenylpyrazol-5-yl ester
	ENT 17,588
	G 22008
	Geigy G-22008
	NSC 404297
	OMS 20
	Pyralan
	Pyrazol-5-ol, 3-methyl-1-phenyl-, dimethyl carbamate
	Pyrazol-5-ol, 3-methyl-1-phenyl-, dimethyl carbamate (ester)
Inchi:	InChI=1S/C13H15N3O2/c1-10-9-12(18-13(17)15(2)3)16(14-10)11-7-5-4-6-8-11/h4-9H,1-
InchiKey:	GEDIWDLJKRKBFT-UHFFFAOYSA-N
Formula:	C13H15N3O2
SMILES:	Cc1cc(OC(=O)N(C)C)n(-c2ccccc2)n1
Mol. weight [g/mol]:	245.28
CAS:	87-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Aqueous Solubility Prediction Method
log10ws	-2.09		Estimated Solubility Method
logp	2.241		Crippen Method
mcvol	188.190	ml/mol	McGowan Method
tf	325.17 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.39	kJ/mol	324.30	NIST Webbook

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=C87478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point