

Carbamic acid, dimethyl-, 3-methyl-1-phenyl-1H-pyrazol-5-yl ester

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-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) pyrolan
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

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
tb	609.98	K	Cheméo Relay (1.0)
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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C87478&Units=SI>

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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