Phenol, 4-(dimethylamino)-3,5-dimethyl-, methylcarbamate (ester)

Other names: Phenol, 4-(dimethylamino)-3,5-dimethyl-, methylcarbamate (ester)
Carbamic acid, methyl-, 4-(dimethylamino)-3,5-xylyl ester
Dowco 139
ENT 25,766
Mexicarbate
Zactran
Zectane
Zectran
Zextran
4-(Dimethylamino)-3,5-Xylyl methylcarbamate
4-Dimethylamino-3,5-dimethylphenyl N-methylcarbamate
4-Dimethylamino-3,5-xylyl N-methylcarbamate
Phenol, 4-(dimethylamino)-3,5-dimethyl-, methylcarbamate
Carbamate, 4-dimethylamino-3,5-xylyl N-methyl-
Carbamic acid, methyl-, 4-(dimethylamino)-3,5-dimethylphenyl ester
4-(Dimethylamine)-3,5-xylyl N-methylcarbamate
4-(Dimethylamino)-3,5-dimethylphenol methylcarbamate
4-(Dimethylamino)-3,5-xylenol, methylcarbamate
4-(N,N-Dimethylamino)-3,5-xylyl N-methylcarbamate
ENT 25766
Methylcarbamic acid, 4-(dimethylamino)-3,5-xylyl ester
Methyl-4-dimethylamino-3,5-xylyl carbamate
Methyl-4-dimethylamino-3,5-xylyl ester of carbamic acid
NCI-C00544
OMS-47
OMS 639
3,5-Xylenol, 4-(dimethylamino)-, methylcarbamate
Carbamic acid, 3,5-dimethyl-4-dimethylaminophenyl ester, N-methyl

Inchi: InChI=1S/C12H18N2O2/c1-8-6-10(16-12(15)13-3)7-9(2)11(8)14(4)5/h6-7H,1-5H3,(H,13,
InchiKey: YNEVBPNZHBAYOA-UHFFFAOYSA-N
Formula: C12H18N2O2
SMILES: CNC(=O)Oc1cc(C)c(N(C)C)c(C)c1
Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source

hfus	30.62	kJ/mol	Joback Method
ie	7.23	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	2.088		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
tb	556.10	K	Cheméo Relay (1.0)
tf	362.06 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.89	J/mol×K	654.48	Joback Method
cpg	496.54	J/mol×K	688.82	Joback Method
cpg	510.35	J/mol×K	723.17	Joback Method
cpg	523.34	J/mol×K	757.51	Joback Method
cpg	535.53	J/mol×K	791.86	Joback Method
cpg	546.94	J/mol×K	826.20	Joback Method
cpg	557.58	J/mol×K	860.54	Joback Method
hfust	18.37	kJ/mol	361.70	NIST Webbook
hfust	18.37	kJ/mol	361.70	NIST Webbook
hfust	18.37	kJ/mol	361.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C315184&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
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