Mexacarbate

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:	C12H16N2O2
SMILES:	CNC(=O)Oc1cc(C)c(N(C)C)c(C)c1
Mol. weight [g/mol]:	220.27
CAS:	315-18-4

Physical Properties

Property code	Value	Unit	Source

gf	99.93	kJ/mol	Joback Method
hf	-212.69	kJ/mol	Joback Method
hfus	30.62	kJ/mol	Joback Method
hvap	64.20	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.088		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	654.48	K	Joback Method
tc	860.54	K	Joback Method
tf	362.06 ± 0.20	K	NIST Webbook
vc	0.676	m3/kmol	Joback Method

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C315184&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume