Carbanolate

Other names:	Phenol, 2-chloro-4,5-dimethyl-, methylcarbamate
	Carbamic acid, methyl-, 6-chloro-3,4-xylyl ester
	Banol
	3,4-Dimethyl-6-chlorophenyl N-methylcarbamate
	6-Chloro-3,4-dimethylphenyl N-methylcarbamate
	6-Chloro-3,4-xylyl methylcarbamate
	Banol tuco sok
	Carbamic acid, methyl-, (2-chloro-4,5-dimethyl)phenyl ester
	Carbamic acid, methyl-, 2-chloro-4,5-xylyl ester
	2-Chloro-4,5-dimethylphenyl methylcarbamate
	Chloroxylam
	6-Chloro-3,4-xylenyl N-methylcarbamate
	2-Chloro-4,5-xylyl N-methylcarbamate
	6-Chloro-3,4-xylyl N-methylcarbamate
	OMS-174
	SOK
	U 12927
	U-17004
	UPJOHN U-12,927
	3,4-Xylyl-6-chloro-N-methylcarbamate
Inchi:	InChI=1S/C10H12ClNO2/c1-6-4-8(11)9(5-7(6)2)14-10(13)12-3/h4-5H,1-3H3,(H,12,13)
InchiKey:	QRTXZGIQTYDABO-UHFFFAOYSA-N
Formula:	C10H12ClNO2
SMILES:	CNC(=O)Oc1cc(C)c(C)cc1Cl
Mol. weight [g/mol]:	213.66
CAS:	671-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-39.62	kJ/mol	Joback Method
hf	-254.68	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.675		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method

tb	633.71	K	Joback Method
tc	852.99	K	Joback Method
tf	421.18	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.82	J/mol×K	633.71	Joback Method
cpg	382.84	J/mol×K	670.26	Joback Method
cpg	394.16	J/mol×K	706.80	Joback Method
cpg	404.79	J/mol×K	743.35	Joback Method
cpg	414.73	J/mol×K	779.89	Joback Method
cpg	423.99	J/mol×K	816.44	Joback Method
cpg	432.56	J/mol×K	852.99	Joback Method

Sources

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=C671045&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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