Chlortoluron

Other names:	3-(3-Chlor-4-methylphenyl)-1,1-dimethylharnstoff
	3-(3-Chloro-4-methylphenyl)-1,1-dimethylurea
	3-(3-Chloro-p-tolyl)-1,1-dimethylurea
	C 2242
	CGA 15646
	Chlorotoluron
	Clortokem
	Dicuran
	Dicuran 500FL
	N,N-Dimethyl-N'-(3-chloro-4-methylphenyl)urea
	N-(3-Chloro-4-methylphenyl)-N',N'-dimethylurea
	Tolurex
	Urea, 3-(3-chloro-p-tolyl)-1,1-dimethyl-
	Urea, N'-(3-chloro-4-methylphenyl)-N,N-dimethyl-
Inchi:	InChI=1S/C10H13ClN2O/c1-7-4-5-8(6-9(7)11)12-10(14)13(2)3/h4-6H,1-3H3,(H,12,14)
InchiKey:	JXCGFZXSOMJFOA-UHFFFAOYSA-N
Formula:	C10H13ClN2O
SMILES:	Cc1ccc(NC(=O)N(C)C)cc1Cl
Mol. weight [g/mol]:	212.68
CAS:	15545-48-9

Physical Properties

Property code	Value	Unit	Source
gf	185.79	kJ/mol	Joback Method
hf	-43.46	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	61.06	kJ/mol	Joback Method
log10ws	-3.46		Aqueous Solubility Prediction Method
log10ws	-3.48		Estimated Solubility Method
logp	2.742		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	618.75	K	Joback Method
tc	836.56	K	Joback Method
tf	421.25	K	Aqueous Solubility Prediction Method

vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.26	J/mol×K	618.75	Joback Method
cpg	397.18	J/mol×K	655.05	Joback Method
cpg	409.24	J/mol×K	691.35	Joback Method
cpg	420.49	J/mol×K	727.66	Joback Method
cpg	430.97	J/mol×K	763.96	Joback Method
cpg	440.71	J/mol×K	800.26	Joback Method
cpg	449.76	J/mol×K	836.56	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C15545489&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