Chlorbromuron

Other names:	1-(3-Chloro-4-bromophenyl)-3-methyl-3-methoxyurea
	1-(4-Bromo-3-chlorophenyl)-3-methoxy-3-methylurea
	3-(4-Bromo-3-Chlorophenyl)-1-methoxy-1-methylurea
	Bromex
	Bromex (herbicide)
	C 6313
	CIBA 6313
	Chlorobromuron
	Maloran
	N-(4-Bromo-3-chlorophenyl)-N'-methoxy-N'-methylurea
	Urea, 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methyl-
	Urea, N'-(4-bromo-3-chlorophenyl)-N-methoxy-N-methyl-
Inchi:	InChI=1S/C9H10BrClN2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,1
InchiKey:	NLYNUTMZTCLNOO-UHFFFAOYSA-N
Formula:	C9H10BrClN2O2
SMILES:	CON(C)C(=O)Nc1ccc(Br)c(Cl)c1
Mol. weight [g/mol]:	293.55
CAS:	13360-45-7

Physical Properties

Property code	Value	Unit	Source
gf	86.69	kJ/mol	Joback Method
hf	-128.71	kJ/mol	Joback Method
hfus	32.72	kJ/mol	Joback Method
hvap	67.68	kJ/mol	Joback Method
log10ws	-3.92		Aqueous Solubility Prediction Method
log10ws	-3.92		Estimated Solubility Method
logp	3.128		Crippen Method
mcvol	171.050	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	684.45	K	Joback Method
tc	914.71	K	Joback Method
tf	370.00 ± 0.20	K	NIST Webbook
tf	370.66 ± 0.20	K	NIST Webbook
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.04	J/mol×K	684.45	Joback Method
cpg	403.69	J/mol×K	722.83	Joback Method
cpg	413.53	J/mol×K	761.20	Joback Method
cpg	422.60	J/mol×K	799.58	Joback Method
cpg	430.94	J/mol×K	837.96	Joback Method
cpg	438.58	J/mol×K	876.34	Joback Method
cpg	445.55	J/mol×K	914.71	Joback Method
hfust	26.54	kJ/mol	369.80	NIST Webbook
hfust	26.54	kJ/mol	369.80	NIST Webbook

Sources

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=C13360457&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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