Metobromuron

Other names: Urea, N'-(4-bromophenyl)-N-methoxy-N-methyl-
Urea, 3-(p-bromophenyl)-1-methoxy-1-methyl-
C 3126
Metbromuron
Patoran
3-(p-Bromophenyl)-1-Methoxy-1-methylurea
3-(4-Bromophenyl)-1-methoxy-1-methylurea
3-(4-Bromphenyl)-1-methoxyharnstoff
N'-(4-Bromophenyl)-N-methoxy-N-methylurea
3-(p-Bromophenyl)-1-methyl-1-methoxyurea
CIBA-3126
Pattonex
Patoran FL
Monobromuron
N-(p-Bromophenyl)-N'-methyl-N'-methoxyurea

Inchi: InChI=1S/C9H11BrN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)

InchiKey: WLFDQEVORAMCIM-UHFFFAOYSA-N

Formula: C9H11BrN2O

SMILES: CON(C)C(=O)Nc1ccc(Br)cc1

Mol. weight [g/mol]: 243.10

CAS: 3060-89-7

Physical Properties

Property code	Value	Unit	Source
gf	108.25	kJ/mol	Joback Method
hf	-101.50	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.474		Crippen Method
mcvol	158.810	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	642.04	K	Joback Method
tc	868.44	K	Joback Method
tf	368.88 ± 0.20	K	NIST Webbook
tf	369.00 ± 0.20	K	NIST Webbook
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.29	J/mol×K	792.98	Joback Method
cpg	422.94	J/mol×K	830.71	Joback Method
cpg	371.94	J/mol×K	642.04	Joback Method
cpg	383.77	J/mol×K	679.77	Joback Method
cpg	394.74	J/mol×K	717.51	Joback Method
cpg	404.91	J/mol×K	755.24	Joback Method
cpg	430.88	J/mol×K	868.44	Joback Method
hfust	24.44	kJ/mol	368.30	NIST Webbook
hfust	24.44	kJ/mol	368.30	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=C3060897&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