Fluometuron

Other names: 1,1-Dimethyl-3-(3-trifluoromethylphenyl)urea
1,1-Dimethyl-3-(«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl) urea
1,1-Dimethyl-3-(Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-m-tolyl) urea
1,1-dimethyl-3-[3-(trifluoromethyl)phenyl]urea
3-(3-Trifluoromethylphenyl)-1,1-dimethylurea
3-(5-Trifluormethylphenyl)-1,1-dimethylharnstoff
3-(m-Trifluoromethylphenyl)-1,1-dimethylurea
C 2059
Ciba 2059
Cotoran
Cotoran multi 50wp
Cottonex
Fluorometuron
Herbicide C-2059
Higalcoton
Kotoran
Lanex
N-(3-Trifluoromethylphenyl)-N',N'-dimethylurea
N-(m-Trifluoromethylphenyl)-N',N'-dimethylurea
NCI-C08695
Pakhtaran
Urea, 1,1-dimethyl-3-(«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-
Urea, 1,1-dimethyl-3-(Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-m-tolyl)-
Urea, N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]-

Inchi: InChI=1S/C10H11F3N2O/c1-15(2)9(16)14-8-5-3-4-7(6-8)10(11,12)13/h3-6H,1-2H3,(H,14

InchiKey: RZILCCPWPBTYDO-UHFFFAOYSA-N

Formula: C10H11F3N2O

SMILES: CN(C)C(=O)Nc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 232.20

CAS: 2164-17-2

Physical Properties

Property code	Value	Unit	Source
gf	-374.24	kJ/mol	Joback Method
hf	-613.33	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method

hvap	52.27	kJ/mol	Joback Method
log10ws	-3.46		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.43		Aqueous Solubility Prediction Method
log10ws	-3.32		Estimated Solubility Method
logp	2.799		Crippen Method
mcvol	154.840	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	570.92	K	Joback Method
tc	766.63	K	Joback Method
tf	436.90	K	Aqueous Solubility Prediction Method
tf	434.80 ± 0.20	K	NIST Webbook
tf	434.00 ± 0.20	K	NIST Webbook
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.15	J/mol×K	734.01	Joback Method
cpg	386.84	J/mol×K	570.92	Joback Method
cpg	399.79	J/mol×K	603.54	Joback Method
cpg	411.85	J/mol×K	636.16	Joback Method
cpg	423.06	J/mol×K	668.77	Joback Method
cpg	433.48	J/mol×K	701.39	Joback Method
cpg	452.12	J/mol×K	766.63	Joback Method
hfust	29.82	kJ/mol	434.10	NIST Webbook

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

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164172&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
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