Urea, N-butyl-N'-(3,4-dichlorophenyl)-N-methyl-

Other names: 1-Butyl-3-(3,4-dichlorophenyl)-1-methylurea
1-n-Butyl-3-(3,4-dichlorophenyl)-1-methylurea
3-(3,4-Dichlorophenyl)-1-methyl-1-butylurea
3-(3,4-Dichlorophenyl)-1-methyl-1-n-butylurea
3-(3,4-Dichlorphenyl)-1-n-butyl-harnstoff
Granurex
Herbalt
Kloben
Kloben neburon
N-Butyl-N'-(3,4-dichlorophenyl)-N-methylurea
Neburea
Neburex
Neburon
Urea, 1-butyl-3-(3,4-dichlorophenyl)-1-methyl-

Inchi: InChI=1S/C12H16Cl2N2O/c1-3-4-7-16(2)12(17)15-9-5-6-10(13)11(14)8-9/h5-6,8H,3-4,7H

InchiKey: CCGPUGMWYLICGL-UHFFFAOYSA-N

Formula: C12H16Cl2N2O

SMILES: CCCCN(C)C(=O)Nc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 275.18

Physical Properties

Property code	Value	Unit	Source
hfus	38.21	kJ/mol	Joback Method
log10ws	-4.77		Aqueous Solubility Prediction Method
log10ws	-4.77		Estimated Solubility Method
logp	4.257		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
tf	373.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	509.49	J/mol×K	701.94	Joback Method
cpg	522.53	J/mol×K	737.62	Joback Method
cpg	534.69	J/mol×K	773.29	Joback Method
cpg	546.02	J/mol×K	808.97	Joback Method
cpg	556.55	J/mol×K	844.64	Joback Method
cpg	566.34	J/mol×K	880.32	Joback Method
cpg	575.42	J/mol×K	915.99	Joback Method

Sources

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C555373&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point