

Neburon

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-Dichlorophenyl)-1-n-butyl-harnstoff
Granurex
Herbalt
Kloben
Kloben neburon
N-Butyl-N'-(3,4-dichlorophenyl)-N-methylurea
Neburea
Neburex

Urea, 1-butyl-3-(3,4-dichlorophenyl)-1-methyl-
Urea, N-butyl-N'-(3,4-dichlorophenyl)-N-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]:

275.17

CAS:

555-37-3

Physical Properties

Property code	Value	Unit	Source
gf	190.70	kJ/mol	Joback Method
hf	-100.48	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	69.90	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
pc	2336.03	kPa	Joback Method
tb	701.94	K	Joback Method
tc	915.99	K	Joback Method
tf	374.60 ± 0.20	K	NIST Webbook

tf	374.86 ± 0.20	K	NIST Webbook
vc	0.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.34	J/mol×K	880.32	Joback Method
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	575.42	J/mol×K	915.99	Joback Method
hfust	27.23	kJ/mol	374.30	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=C555373&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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