Tolbutamide

Other names:

1-Butyl-3-(p-methylphenylsulfonyl)urea
1-Butyl-3-(p-tolylsulfonyl)urea
1-Butyl-3-(para-tolylsulfonyl)-urea
1-Butyl-3-tosylurea
1-p-Toluenesulfonyl-3-butylurea
3-(P-tolyl-4-sulfonyl)-1-butyl urea (tolbutamide)
3-(p-Tolyl-4-sulfonyl)-1-butylurea
Aglicid
Arkozal
Artosin
Artozin
Benzenesulfonamide, N-[(butylamino)carbonyl]-4-methyl-
Butamid
Butamide
D 860
Diaben
Diabetamid
Diabetol
Diabuton
Diasulfon
Dirastan
Dolipol
Drabet
Glyconon
HLS 831
Ipoglicone
Mobenol
N-(4-Methylbenzenesulfonyl)-N'-butylurea
N-(4-Methylphenylsulfonyl)-N'-butylurea
N-(Sulfonyl-p-methylbenzene)-N'-N-butylurea
N-(n-Butyl)-N'-p-toluene-sulfonylurea
N-(p-Methylbenzenesulfonyl)-N'-butylurea
N-(p-Tolylsulfonyl)-N'-butylcarbamide
N-4-Methylbenzolsulfonyl-N-butylurea
N-Butyl-N'-(4-methylphenylsulfonyl)urea
N-Butyl-N'-(p-tolylsulfonyl)urea
N-Butyl-N'-p-toluenesulfonylurea
N-Butyl-N'-toluene-p-sulfonylurea
N-[(butylamino)carbonyl]-4-methylbenzenesulfonamide
N-n-Butyl-N'-tosylurea

NCI-C01763
Orabet
Oralin
Orezan
Orinase
Orinaz
Oterben
Pramidex
Rastinon
SK-tolbutamide
Tolbusal
Tolbutamid
Toluina
Tolumid
Tolumide
Toluvan
Tolylsulfonylbutylurea
U-2043
Urea, 1-butyl-3-(p-tolylsulfonyl)-
Willbutamide

Inchi: InChI=1S/C12H18N2O3S/c1-3-4-9-13-12(15)14-18(16,17)11-7-5-10(2)6-8-11/h5-8H,3-4,

InchiKey: JLRGJRBPOGGCBT-UHFFFAOYSA-N

Formula: C12H18N2O3S

SMILES: CCCCNC(=O)NS(=O)(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 270.35

CAS: 64-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-265.74	kJ/mol	Joback Method
hf	-524.94	kJ/mol	Joback Method
hfus	43.66	kJ/mol	Joback Method
hvap	83.50	kJ/mol	Joback Method
log10ws	-3.46		Aqueous Solubility Prediction Method
log10ws	-3.39		Aqueous Solubility Prediction Method
logp	1.783		Crippen Method
mcvol	205.800	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method

tb	707.61	K	Joback Method
tc	910.31	K	Joback Method
tf	401.77	K	Aqueous Solubility Prediction Method
tf	401.77	K	Aqueous Solubility Prediction Method
tf	400.00 ± 1.00	K	NIST Webbook
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.97	J/mol×K	808.96	Joback Method
cpg	609.05	J/mol×K	842.75	Joback Method
cpg	619.22	J/mol×K	876.53	Joback Method
cpg	559.03	J/mol×K	707.61	Joback Method
cpg	572.98	J/mol×K	741.39	Joback Method
cpg	585.95	J/mol×K	775.18	Joback Method
cpg	628.49	J/mol×K	910.31	Joback Method
hfust	27.20	kJ/mol	400.20	NIST Webbook
hfust	25.60	kJ/mol	404.80	NIST Webbook
hfust	25.61	kJ/mol	404.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64777&Units=SI

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

Solubility of Tolbutamide and Chlorpropamide in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/acs.jced.8b00050

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

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

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