3-(p-Tolyl-4-sulfonyl)-1-butyl urea

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
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
	benzenesulfonamide, N-[(butylamino)carbonyl]-4-methyl-
	tolbutamide
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

Physical Properties

Property code	Value	Unit	Source
hfus	43.66	kJ/mol	Joback Method
log10ws	-3.39		Aqueous Solubility Prediction Method
log10ws	-3.46		Aqueous Solubility Prediction Method
logp	1.783		Crippen Method
mcvol	205.800	ml/mol	McGowan 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

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	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	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

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

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

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):

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

Cheméo Relay (1.0, beta):

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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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