Phenylbutazone

Other names:

1,2-Diphenyl-3,5-dioxo-4-butylpyrazolidine
1,2-Diphenyl-3,5-dioxo-4-n-butylpyrazolidine
1,2-Diphenyl-4-butyl-3,5-dioxopyrazolidine
1,2-Diphenyl-4-butyl-3,5-pyrazolidinedione
3,5-Dioxo-1,2-diphenyl-4-n-butyl-pyrazolidin
3,5-Dioxo-1,2-diphenyl-4-n-butylpyrazolidine
3,5-Pyrazolidinedione, 4-butyl-1,2-diphenyl-
4-Butyl-1,2-diphenyl-3,5-dioxopyrazolidine
4-Butyl-1,2-diphenyl-3,5-pyrazolidinedione
4-Butyl-1,2-diphenylpyrazolidine-3,5-dione
4-n-Butyl-1,2-diphenyl-3,5-pyrazolidinedione
A 7514
Alindor
Alkabutazona
Alkazone
Alqoverin
Anerval
Anpuzone
Antadol
Anuspiramin
Arthrizon
Artrizin
Artrizone
Artropan
Azdid
Azobutyl
Azolid
B.t.z.
Benzone
Betazed
Bizolin 200
Bunetzone
Busone
Butacompren
Butacote
Butadion
Butadiona
Butadione
Butagesic
Butalan

Butalgina
Butalidon
Butaluy
Butaphen
Butapirazol
Butapirazole
Butapyrazole
Butarecbon
Butartril
Butartrina
Butazina
Butazolidin
Butazolidine
Butazona
Butazone
Bute
Butidiona
Butiwas-Simple
Butone
Butoz
Butylpyrin
Buvetzone
Buzon
Chembutazone
DA-192
Digibutina
Diossidone
Diozol
Diphebuzol
Diphenylbutazone
Ecobutazone
Elmedal
Equi bute
Equipalazone
Eributazone
Esteve
Febuzina
Fenartil
Fenibutal
Fenibutasan
Fenibutazona
Fenibutol
Fenilbutazona

Fenilbutina
Fenilbutine
Fenilidina
Fenotone
Fenylbutazon
Flexazone
G 13,871
Ia-But
Intalbut
Intrabutazone
Intrazone
Ipsoflame
Kadol
Lingel
Malgesic
Mephabutazon
Mephabutazone
Merizone
NCI-C55414
Nadazone
Nadozone
Neo-zoline
Novophenyl
PBZ
Phebuzin
Phebuzine
Phen-Buta
Phenbutazol
Phenopyrine
Phenyl-Mobuzon
Phenylbutaz
Phenylbutazonum
Phenyzone
Pirarreumol B
Praecirheumin
Pyrabutol
Pyrazolidin
R-3-ZON
Rectofasa
Reudo
Reudox
Reumasyl
Reumazin

Reumazol
Reumune
Reumuzol
Reupolar
Robizon-V
Robizone
Rubatone
Scanbutazone
Schemergin
Shigrodin
Tazone
Tencodyne
Tetnor
Tevcodyne
Therazone
Ticinil
Todalgil
USAF GE-15
Uzone
VAC-10
Wescozone
Zolaphen
Zolidinum
Zorane

Inchi: InChI=1S/C19H20N2O2/c1-2-3-14-17-18(22)20(15-10-6-4-7-11-15)21(19(17)23)16-12-8-

InchiKey: VYMDGNCVAMGZFE-UHFFFAOYSA-N

Formula: C19H20N2O2

SMILES: CCCCC1C(=O)N(c2ccccc2)N(c2ccccc2)C1=O

Mol. weight [g/mol]: 308.37

CAS: 50-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Aqueous Solubility Prediction Method
log10ws	-3.81		Estimated Solubility Method
logp	3.788		Crippen Method
mcvol	243.290	ml/mol	McGowan Method
rinpol	2404.00		NIST Webbook

rinpol	2333.00		NIST Webbook
rinpol	2404.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2443.60		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2352.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2443.60		NIST Webbook
tf	377.00 ± 1.00	K	NIST Webbook
tf	472.22	K	Aqueous Solubility Prediction Method

Sources

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=C50339&Units=SI

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

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point