3,5-Pyrazolidinedione, 4-butyl-1-(4-hydroxyphenyl)-2-phenyl-

Other names:

1-(p-Hydroxyphenyl)-2-phenyl-3,5-dioxo-4-N-butylpyrazolidine
1-(p-Hydroxyphenyl)-2-phenyl-4-butyl-3,5-pyrazolidinedione
1-Phenyl-2-(p-hydroxyphenyl)-3,5-dioxo-4-butylpyrazolidine
1-Phenyl-2-(p-hydroxyphenyl)-3,5-dioxo-4-n-butylpyrazolidine
3,5-Dioxo-1-phenyl-2-(p-hydroxyphenyl)-4-N-butylpyrazolidene
3,5-Pyrazolidinedione, 4-butyl-1-(p-hydroxyphenyl)-2-phenyl-
4-Butyl-1-(4-hydroxyphenyl)-2-phenyl-3,5-pyrazolidinedione
4-Butyl-1-(p-hydroxyphenyl)-2-phenyl-3,5-pyrazolidinedione
4-Butyl-2-(4-hydroxyphenyl)-1-phenyl-3,5-dioxopyrazolidine
4-Butyl-2-(p-hydroxyphenyl)-1-phenyl-3,5-pyrazolidinedione
Artroflog
BM 1
Butaflogin
Butanova
Butapirone
Butazonic
Butilene
Californit
Crovaril
Deflogin
Etrozolidina
Flamaril
Flanaril
Flogal
Floghene
Flogistin
Flogitolo
Flogodin
Flogoril
Flogostop
Flopirina
Frabel
G 27202
Idrobutazina
Infamil
Infammil
Ipabutona
Iridil
Isobutazina
Isobutil

Metabolite I
Mysite
Neo-Farmadol
Neofen
Offitril
Optimal
Oxalid
Oxazolidin
Oxazolidin-Geigy
Oxi-Fenibutol
Oxibutol
Oxifenylbutazon
Oxiphenbutazone
Oxybuton
Oxyphenobutazone
Oxyphentamin
Oxyphenylbutazone
Pirabutina
Piraflogin
Poliflogil
Rapostan
Remazin
Reumox
Romaxin
Rumapax
Suganril
Tandacote
Tandalgesic
Tandearil
Tanderal
Tanderil
Telidal
Tendearil
USAF GE-14
Valioil
Visubutina
oxyphenbutazone
p-Hydroxyphenylbutazone
p-Oxyphenylbutazone

Inchi: InChI=1S/C19H20N2O3/c1-2-3-9-17-18(23)20(14-7-5-4-6-8-14)21(19(17)24)15-10-12-16

InchiKey: HFHZKZSRXITVMK-UHFFFAOYSA-N

Formula: C19H20N2O3

SMILES: CCCCC1C(=O)N(c2ccccc2)N(c2ccc(O)cc2)C1=O

Mol. weight [g/mol]: 324.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Aqueous Solubility Prediction Method
log10ws	-3.73		Estimated Solubility Method
logp	3.493		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
tf	442.28	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
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=C129204&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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