Bentazone

Other names: 1H-2,1,3-Benzothiadiazin-4(3H)-one, 3-(1-methylethyl)-, 2,2-dioxide
1H-2,1,3-Benzothiadiazin-4(3H)-one, 3-isopropyl-, 2,2-dioxide
3-(1-Methylethyl)-1H-2,1,3-benzothia-diazin-4(3H)-one 2,2-dioxide
3-Isopropyl-1H-2,1,3-benzothiadiazin-4(3H)-one-2,2-dioxide
3-Isopropyl-2,1,3-benzothiadiazinon-(4)-2,2-dioxid
3-Isopropyl-4-oxo-2,1,3-benzothiadiazine 2,2-dioxide
Adagio
BAS 351-07H
BAS 3510
BAS 3510H
BAS 3512H
BAS 3517H
BAS 351H
Basagran
Basagran 480
Bendioxide
Bentazon
Leader
Pentazone

Inchi: InChI=1S/C10H12N2O3S/c1-7(2)12-10(13)8-5-3-4-6-9(8)11-16(12,14)15/h3-7,11H,1-2H3

InchiKey: ZOMSMJKLGFBRBS-UHFFFAOYSA-N

Formula: C10H12N2O3S

SMILES: CC(C)N1C(=O)c2ccccc2NS1(=O)=O

Mol. weight [g/mol]: 240.28

CAS: 25057-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Aqueous Solubility Prediction Method
logp	1.208		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tf	412.81 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.77	kJ/mol	412.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25057890&Units=SI

Legend

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point