

Bendroflumethiazide

Other names:	1,1-dioxo-3-(phenylmethyl)-6-(trifluoromethyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine-7
Inchi:	InChI=1S/C15H14F3N3O4S2/c16-15(17,18)10-7-11-13(8-12(10)26(19,22)23)27(24,25)2
InchiKey:	HDWIHXWEUNVBIY-UHFFFAOYSA-N
Formula:	C15H14F3N3O4S2
SMILES:	NS(=O)(=O)c1cc2c(cc1C(F)(F)F)NC(Cc1ccccc1)NS2(=O)=O
Mol. weight [g/mol]:	421.42

Physical Properties

Property code	Value	Unit	Source
gf	-950.06	kJ/mol	Joback Method
hf	-1238.62	kJ/mol	Joback Method
hfus	66.04	kJ/mol	Joback Method
hvap	112.28	kJ/mol	Joback Method
log10ws	-3.59		Aqueous Solubility Prediction Method
log10ws	-3.89		Aqueous Solubility Prediction Method
log10ws	-3.59		Estimated Solubility Method
logp	1.625		Crippen Method
mcvol	255.260	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
tb	860.73	K	Joback Method
tc	1088.40	K	Joback Method
tf	787.31	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.43	J/molxK	860.73	Joback Method
cpg	763.86	J/molxK	898.68	Joback Method
cpg	773.93	J/molxK	936.62	Joback Method
cpg	782.68	J/molxK	974.57	Joback Method
cpg	790.16	J/molxK	1012.51	Joback Method

cpg	796.43	J/mol×K	1050.46	Joback Method
cpg	801.54	J/mol×K	1088.40	Joback 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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
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

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