Bumetanide

Inchi: InChI=1S/C17H20N2O5S/c1-2-3-9-19-14-10-12(17(20)21)11-15(25(18,22)23)16(14)24-1
InchiKey: MAEIEVLCKWDQJH-UHFFFAOYSA-N
Formula: C17H20N2O5S
SMILES: CCCCNc1cc(C(=O)O)cc(S(N)(=O)=O)c1Oc1ccccc1
Mol. weight [g/mol]: 364.42

Physical Properties

Property code	Value	Unit	Source
gf	-395.25	kJ/mol	Joback Method
hf	-718.68	kJ/mol	Joback Method
hfus	55.25	kJ/mol	Joback Method
hvap	121.52	kJ/mol	Joback Method
log10ws	-3.56		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.12		Aqueous Solubility Prediction Method
logp	3.036		Crippen Method
mcvol	264.230	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	995.61	K	Joback Method
tc	1224.23	K	Joback Method
tf	503.65	K	Aqueous Solubility Prediction Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.45	J/mol×K	995.61	Joback Method
cpg	825.81	J/mol×K	1033.71	Joback Method
cpg	832.81	J/mol×K	1071.82	Joback Method
cpg	838.48	J/mol×K	1109.92	Joback Method
cpg	842.84	J/mol×K	1148.02	Joback Method
cpg	845.92	J/mol×K	1186.13	Joback Method

cpg	847.74	J/mol×K	1224.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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