Xipamide

Other names: 4-chloro-N-(2,6-dimethylphenyl)-2-hydroxy-5-sulfamoylbenzamide
Inchi: InChI=1S/C15H15ClN2O4S/c1-8-4-3-5-9(2)14(8)18-15(20)10-6-13(23(17,21)22)11(16)7-
InchiKey: MTZBBNMLMNBNJL-UHFFFAOYSA-N
Formula: C15H15ClN2O4S
SMILES: Cc1cccc(C)c1NC(=O)c1cc(S(N)(=O)=O)c(Cl)cc1O
Mol. weight [g/mol]: 354.81

Physical Properties

Property code	Value	Unit	Source
gf	-346.45	kJ/mol	Joback Method
hf	-597.47	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	116.04	kJ/mol	Joback Method
log10ws	-3.79		Aqueous Solubility Prediction Method
log10ws	-3.79		Estimated Solubility Method
logp	2.562		Crippen Method
mcvol	242.420	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	958.28	K	Joback Method
tc	1204.82	K	Joback Method
tf	727.78	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.90	J/mol×K	958.28	Joback Method
cpg	705.64	J/mol×K	999.37	Joback Method
cpg	714.56	J/mol×K	1040.46	Joback Method
cpg	722.76	J/mol×K	1081.55	Joback Method
cpg	730.33	J/mol×K	1122.64	Joback Method
cpg	737.34	J/mol×K	1163.73	Joback Method

cpg	743.88	J/mol×K	1204.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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