hydroflumethiazide

Inchi: InChI=1S/C8H8F3N3O4S2/c9-8(10,11)4-1-5-7(2-6(4)19(12,15)16)20(17,18)14-3-13-5/h1
InchiKey: DMDGGSIALPNSEE-UHFFFAOYSA-N
Formula: C8H8F3N3O4S2
SMILES: NS(=O)(=O)c1cc2c(cc1C(F)(F)F)NCNS2(=O)=O
Mol. weight [g/mol]: 331.30

Physical Properties

Property code	Value	Unit	Source
gf	-1113.70	kJ/mol	Joback Method
hf	-1310.33	kJ/mol	Joback Method
hfus	52.80	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Joback Method
log10ws	-3.30		Aqueous Solubility Prediction Method
logp	0.014		Crippen Method
mcvol	180.390	ml/mol	McGowan Method
pc	6567.04	kPa	Joback Method
tb	678.56	K	Joback Method
tc	892.43	K	Joback Method
tf	545.03	K	Aqueous Solubility Prediction Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.47	J/mol×K	678.56	Joback Method
cpg	481.68	J/mol×K	714.20	Joback Method
cpg	491.92	J/mol×K	749.85	Joback Method
cpg	501.23	J/mol×K	785.49	Joback Method
cpg	509.62	J/mol×K	821.14	Joback Method
cpg	517.11	J/mol×K	856.78	Joback Method
cpg	523.72	J/mol×K	892.43	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
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