4-Chloro-N-(2-hydroxypropionyl)-benzenesulfona
O-trifluoroacetyl-

Inchi: InChI=1S/C11H9ClF3NO5S/c1-6(21-10(18)11(13,14)15)9(17)16-22(19,20)8-4-2-7(12)3-5
InchiKey: XJVUBPGZNBCJIR-UHFFFAOYSA-N
Formula: C11H9ClF3NO5S
SMILES: CC(OC(=O)C(F)(F)F)C(=O)NS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 359.71

Physical Properties

Property code	Value	Unit	Source
gf	-1193.43	kJ/mol	Joback Method
hf	-1420.67	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.639		Crippen Method
mcvol	206.720	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	742.42	K	Joback Method
tc	945.31	K	Joback Method
tf	485.09	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.58	J/mol×K	742.42	Joback Method
cpg	555.57	J/mol×K	776.24	Joback Method
cpg	564.64	J/mol×K	810.05	Joback Method
cpg	572.80	J/mol×K	843.87	Joback Method
cpg	580.09	J/mol×K	877.68	Joback Method
cpg	586.51	J/mol×K	911.50	Joback Method
cpg	592.10	J/mol×K	945.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume