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

Inchi: InChI=1S/C11H12ClNO5S/c1-7(18-8(2)14)11(15)13-19(16,17)10-5-3-9(12)4-6-10/h3-7H,

InchiKey: YJPRGEJXWHQENP-UHFFFAOYSA-N

Formula: C11H12ClNO5S

SMILES: CC(=O)OC(C)C(=O)NS(=O)(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 305.74

Physical Properties

Property code	Value	Unit	Source
gf	-611.84	kJ/mol	Joback Method
hf	-823.59	kJ/mol	Joback Method
hfus	39.43	kJ/mol	Joback Method
hvap	87.99	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.097		Crippen Method
mcvol	201.410	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	747.84	K	Joback Method
tc	964.31	K	Joback Method
tf	480.90	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.40	J/mol×K	747.84	Joback Method
cpg	530.64	J/mol×K	783.92	Joback Method
cpg	540.86	J/mol×K	820.00	Joback Method
cpg	550.06	J/mol×K	856.08	Joback Method
cpg	558.26	J/mol×K	892.16	Joback Method
cpg	565.44	J/mol×K	928.23	Joback Method
cpg	571.62	J/mol×K	964.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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