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

Inchi: InChI=1S/C10H12ClNO4S/c1-7(16-2)10(13)12-17(14,15)9-5-3-8(11)4-6-9/h3-7H,1-2H3,(

InchiKey: YXMIQDWHNXBYRS-UHFFFAOYSA-N

Formula: C10H12ClNO4S

SMILES: COC(C)C(=O)NS(=O)(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 277.73

Physical Properties

Property code	Value	Unit	Source
gf	-491.34	kJ/mol	Joback Method
hf	-690.37	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.180		Crippen Method
mcvol	185.750	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	2005.00		NIST Webbook
tb	671.09	K	Joback Method
tc	884.61	K	Joback Method
tf	419.70	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.93	J/mol×K	671.09	Joback Method
cpg	468.37	J/mol×K	706.68	Joback Method
cpg	479.90	J/mol×K	742.26	Joback Method
cpg	490.51	J/mol×K	777.85	Joback Method
cpg	500.21	J/mol×K	813.44	Joback Method
cpg	508.99	J/mol×K	849.02	Joback Method
cpg	516.87	J/mol×K	884.61	Joback Method

Sources

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=U374381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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