N-(2-Hydroxy-propionyl)-4-methyl-benzenesulfona
O-methyl-

Inchi: InChI=1S/C11H15NO4S/c1-8-4-6-10(7-5-8)17(14,15)12-11(13)9(2)16-3/h4-7,9H,1-3H3,(
InchiKey: RSDRHGLMKFCKID-UHFFFAOYSA-N
Formula: C11H15NO4S
SMILES: COC(C)C(=O)NS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 257.31

Physical Properties

Property code	Value	Unit	Source
gf	-470.99	kJ/mol	Joback Method
hf	-695.27	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	76.86	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	0.835		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
tb	656.54	K	Joback Method
tc	863.47	K	Joback Method
tf	401.05	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.87	J/mol×K	656.54	Joback Method
cpg	494.90	J/mol×K	691.03	Joback Method
cpg	508.00	J/mol×K	725.52	Joback Method
cpg	520.18	J/mol×K	760.00	Joback Method
cpg	531.44	J/mol×K	794.49	Joback Method
cpg	541.78	J/mol×K	828.98	Joback Method
cpg	551.19	J/mol×K	863.47	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=U374250&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