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

O-acetyl-

Inchi: InChI=1S/C12H15NO5S/c1-8-4-6-11(7-5-8)19(16,17)13-12(15)9(2)18-10(3)14/h4-7,9H,1

InchiKey: CELNKQZYEGTTMP-UHFFFAOYSA-N

Formula: C12H15NO5S

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

Mol. weight [g/mol]: 285.32

Physical Properties

Property code	Value	Unit	Source
gf	-591.49	kJ/mol	Joback Method
hf	-828.49	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	0.752		Crippen Method
mcvol	203.260	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	733.29	K	Joback Method
tc	943.79	K	Joback Method
tf	462.25	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.34	J/mol×K	733.29	Joback Method
cpg	561.15	J/mol×K	768.37	Joback Method
cpg	572.93	J/mol×K	803.46	Joback Method
cpg	583.69	J/mol×K	838.54	Joback Method
cpg	593.43	J/mol×K	873.62	Joback Method
cpg	602.15	J/mol×K	908.70	Joback Method
cpg	609.84	J/mol×K	943.79	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=U374742&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