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

Inchi: InChI=1S/C10H13NO4S/c1-7-3-5-9(6-4-7)16(14,15)11-10(13)8(2)12/h3-6,8,12H,1-2H3,(H
InchiKey: UGYBMUFRMSFALF-UHFFFAOYSA-N
Formula: C10H13NO4S
SMILES: Cc1ccc(S(=O)(=O)NC(=O)C(C)O)cc1
Mol. weight [g/mol]: 243.28
CAS: 91013-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-511.23	kJ/mol	Joback Method
hf	-694.64	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.181		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	703.42	K	Joback Method
tc	902.96	K	Joback Method
tf	428.37	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.24	J/mol×K	703.42	Joback Method
cpg	468.21	J/mol×K	736.68	Joback Method
cpg	478.38	J/mol×K	769.93	Joback Method
cpg	487.77	J/mol×K	803.19	Joback Method
cpg	496.39	J/mol×K	836.45	Joback Method
cpg	504.25	J/mol×K	869.70	Joback Method
cpg	511.38	J/mol×K	902.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91013535&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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