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

Inchi: InChI=1S/C11H15NO4S/c1-8-4-6-10(7-5-8)17(15,16)12(3)11(14)9(2)13/h4-7,9,13H,1-3H

InchiKey: NHLMRXSPXFBDLY-UHFFFAOYSA-N

Formula: C11H15NO4S

SMILES: Cc1ccc(S(=O)(=O)N(C)C(=O)C(C)O)cc1

Mol. weight [g/mol]: 257.31

Physical Properties

Property code	Value	Unit	Source
gf	-481.42	kJ/mol	Joback Method
hf	-701.22	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	0.523		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1941.00		NIST Webbook
rinpol	1941.00		NIST Webbook
tb	688.57	K	Joback Method
tc	883.24	K	Joback Method
tf	419.45	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.50	J/mol×K	688.57	Joback Method
cpg	508.65	J/mol×K	721.01	Joback Method
cpg	519.96	J/mol×K	753.46	Joback Method
cpg	530.46	J/mol×K	785.90	Joback Method
cpg	540.17	J/mol×K	818.35	Joback Method
cpg	549.10	J/mol×K	850.79	Joback Method
cpg	557.28	J/mol×K	883.24	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=U374394&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