N-(2-Hydroxy-1-phenyl-ethyl)-benzenesulfonamid

Inchi: InChI=1S/C14H15NO3S/c16-11-14(12-7-3-1-4-8-12)15-19(17,18)13-9-5-2-6-10-13/h1-10
InchiKey: YQUFKSRAKRZOFV-UHFFFAOYSA-N
Formula: C14H15NO3S
SMILES: O=S(=O)(NC(CO)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 277.34
CAS: 919706-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-226.59	kJ/mol	Joback Method
hf	-416.62	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	92.67	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.698		Crippen Method
mcvol	204.540	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	762.77	K	Joback Method
tc	978.22	K	Joback Method
tf	437.42	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.30	J/mol×K	762.77	Joback Method
cpg	578.81	J/mol×K	798.68	Joback Method
cpg	590.22	J/mol×K	834.59	Joback Method
cpg	600.58	J/mol×K	870.50	Joback Method
cpg	609.93	J/mol×K	906.41	Joback Method
cpg	618.31	J/mol×K	942.31	Joback Method
cpg	625.78	J/mol×K	978.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C919706175&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

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