N-(2-Hydroxy-1-phenyl-ethyl)-benzenesulfonamid N,O-dimethyl-

Inchi: InChI=1S/C16H19NO3S/c1-17(21(18,19)15-11-7-4-8-12-15)16(13-20-2)14-9-5-3-6-10-14
InchiKey: PIQFTHAKJAFVON-UHFFFAOYSA-N
Formula: C16H19NO3S
SMILES: COCC(c1ccccc1)N(C)S(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 305.39

Physical Properties

Property code	Value	Unit	Source
gf	-156.54	kJ/mol	Joback Method
hf	-423.83	kJ/mol	Joback Method
hfus	37.34	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.695		Crippen Method
mcvol	232.720	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook
tb	701.04	K	Joback Method
tc	920.05	K	Joback Method
tf	401.18	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.30	J/mol×K	701.04	Joback Method
cpg	646.73	J/mol×K	737.54	Joback Method
cpg	662.78	J/mol×K	774.04	Joback Method
cpg	677.49	J/mol×K	810.55	Joback Method
cpg	690.91	J/mol×K	847.05	Joback Method
cpg	703.07	J/mol×K	883.55	Joback Method
cpg	714.03	J/mol×K	920.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374422&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