N-(2-Hydroxy-2-phenyl-ethyl)-4-methyl-benzenesu
N,O-dimethyl-

Inchi: InChI=1S/C17H21NO3S/c1-14-9-11-16(12-10-14)22(19,20)18(2)13-17(21-3)15-7-5-4-6-8

InchiKey: WCEMHQUXXSJOCV-UHFFFAOYSA-N

Formula: C17H21NO3S

SMILES: COC(CN(C)S(=O)(=O)c1ccc(C)cc1)c1ccccc1

Mol. weight [g/mol]: 319.42

Physical Properties

Property code	Value	Unit	Source
gf	-157.75	kJ/mol	Joback Method
hf	-455.94	kJ/mol	Joback Method
hfus	39.54	kJ/mol	Joback Method
hvap	81.35	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.003		Crippen Method
mcvol	246.810	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	728.90	K	Joback Method
tc	945.38	K	Joback Method
tf	424.97	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.69	J/mol×K	728.90	Joback Method
cpg	701.06	J/mol×K	764.98	Joback Method
cpg	717.07	J/mol×K	801.06	Joback Method
cpg	731.75	J/mol×K	837.14	Joback Method
cpg	745.15	J/mol×K	873.22	Joback Method
cpg	757.29	J/mol×K	909.30	Joback Method
cpg	768.23	J/mol×K	945.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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