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

Inchi: InChI=1S/C16H19NO3S/c1-13-8-10-15(11-9-13)21(18,19)17-12-16(20-2)14-6-4-3-5-7-14

InchiKey: ZUVKONYUKGMKQC-UHFFFAOYSA-N

Formula: C16H19NO3S

SMILES: COC(CNS(=O)(=O)c1ccc(C)cc1)c1ccccc1

Mol. weight [g/mol]: 305.39

Physical Properties

Property code	Value	Unit	Source
gf	-187.56	kJ/mol	Joback Method
hf	-449.36	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.661		Crippen Method
mcvol	232.720	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	743.75	K	Joback Method
tc	965.45	K	Joback Method
tf	433.89	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.78	J/mol×K	743.75	Joback Method
cpg	660.87	J/mol×K	780.70	Joback Method
cpg	675.62	J/mol×K	817.65	Joback Method
cpg	689.07	J/mol×K	854.60	Joback Method
cpg	701.23	J/mol×K	891.55	Joback Method
cpg	712.15	J/mol×K	928.50	Joback Method
cpg	721.86	J/mol×K	965.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374829&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