N-(2-Acetyloxy-1-phenyl-ethyl)-benzenesulfonami

Inchi: InChI=1S/C16H17NO4S/c1-13(18)21-12-16(14-8-4-2-5-9-14)17-22(19,20)15-10-6-3-7-11
InchiKey: BQPCOGFDEPVRIR-UHFFFAOYSA-N
Formula: C16H17NO4S
SMILES: CC(=O)OCC(NS(=O)(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 319.38

Physical Properties

Property code	Value	Unit	Source
gf	-306.85	kJ/mol	Joback Method
hf	-550.47	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.269		Crippen Method
mcvol	234.290	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	792.64	K	Joback Method
tc	1019.18	K	Joback Method
tf	471.30	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.32	J/mol×K	792.64	Joback Method
cpg	675.36	J/mol×K	830.40	Joback Method
cpg	688.01	J/mol×K	868.15	Joback Method
cpg	699.32	J/mol×K	905.91	Joback Method
cpg	709.33	J/mol×K	943.67	Joback Method
cpg	718.07	J/mol×K	981.43	Joback Method
cpg	725.57	J/mol×K	1019.18	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=U374419&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