Probenazole

Other names: 1,2-Benzisothiazole, 3-(2-propen-1-yloxy)-, 1,1-dioxide
Inchi: InChI=1S/C10H9NO3S/c1-2-7-14-10-8-5-3-4-6-9(8)15(12,13)11-10/h2-6H,1,7H2
InchiKey: WHHIPMZEDGBUCC-UHFFFAOYSA-N
Formula: C10H9NO3S
SMILES: C=CCOC1=NS(=O)(=O)c2ccccc21
Mol. weight [g/mol]: 223.25
CAS: 27605-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-137.29	kJ/mol	Joback Method
hf	-271.00	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.338		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
rinpol	1950.00		NIST Webbook
tb	575.04	K	Joback Method
tc	796.45	K	Joback Method
tf	456.48	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.12	J/mol×K	575.04	Joback Method
cpg	373.80	J/mol×K	611.94	Joback Method
cpg	386.54	J/mol×K	648.84	Joback Method
cpg	398.37	J/mol×K	685.75	Joback Method
cpg	409.32	J/mol×K	722.65	Joback Method
cpg	419.41	J/mol×K	759.55	Joback Method
cpg	428.66	J/mol×K	796.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27605761&Units=SI

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