Probenecid Me, #1

Inchi: InChI=1S/C14H21NO4S/c1-4-10-15(11-5-2)20(17,18)13-8-6-12(7-9-13)14(16)19-3/h6-9H
InchiKey: YLVGRYMYFMKKCB-UHFFFAOYSA-N
Formula: C14H21NO4S
SMILES: CCCN(CCC)S(=O)(=O)c1ccc(C(=O)OC)cc1
Mol. weight [g/mol]: 299.39

Physical Properties

Property code	Value	Unit	Source
gf	-421.90	kJ/mol	Joback Method
hf	-737.85	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	79.53	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.284		Crippen Method
mcvol	229.870	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2139.00		NIST Webbook
tb	687.89	K	Joback Method
tc	881.54	K	Joback Method
tf	429.67	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.48	J/mol×K	687.89	Joback Method
cpg	638.25	J/mol×K	720.17	Joback Method
cpg	653.02	J/mol×K	752.44	Joback Method
cpg	666.82	J/mol×K	784.72	Joback Method
cpg	679.65	J/mol×K	816.99	Joback Method
cpg	691.53	J/mol×K	849.27	Joback Method
cpg	702.47	J/mol×K	881.54	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=R40461&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