Hydroxyacetone p-Toluenesulfonate

Inchi: InChI=1S/C10H12O4S/c1-8-3-5-10(6-4-8)15(12,13)14-7-9(2)11/h3-6H,7H2,1-2H3
InchiKey: PMXQYMFAWGAWGF-UHFFFAOYSA-N
Formula: C10H12O4S
SMILES: CC(=O)COS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 228.26

Physical Properties

Property code	Value	Unit	Source
gf	-566.36	kJ/mol	Joback Method
hf	-722.82	kJ/mol	Joback Method
hfus	29.47	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.289		Crippen Method
mcvol	163.530	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1778.00		NIST Webbook
tb	583.93	K	Joback Method
tc	790.02	K	Joback Method
tf	352.12	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.54	J/mol×K	583.93	Joback Method
cpg	393.94	J/mol×K	618.28	Joback Method
cpg	406.57	J/mol×K	652.63	Joback Method
cpg	418.44	J/mol×K	686.98	Joback Method
cpg	429.54	J/mol×K	721.32	Joback Method
cpg	439.85	J/mol×K	755.67	Joback Method
cpg	449.39	J/mol×K	790.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412885&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