N-(2-Hydroxy-propionyl)-4-methyl-benzenesulfona O-trifluoroacetyl-

Inchi: InChI=1S/C12H12F3NO5S/c1-7-3-5-9(6-4-7)22(19,20)16-10(17)8(2)21-11(18)12(13,14)1

InchiKey: ZESVQAAZGWYBNE-UHFFFAOYSA-N

Formula: C12H12F3NO5S

SMILES: Cc1ccc(S(=O)(=O)NC(=O)C(C)OC(=O)C(F)(F)F)cc1

Mol. weight [g/mol]: 339.29

Physical Properties

Property code	Value	Unit	Source
gf	-1173.08	kJ/mol	Joback Method
hf	-1425.57	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	1.294		Crippen Method
mcvol	208.570	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	727.87	K	Joback Method
tc	925.30	K	Joback Method
tf	466.44	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.51	J/mol×K	727.87	Joback Method
cpg	586.03	J/mol×K	760.77	Joback Method
cpg	596.61	J/mol×K	793.68	Joback Method
cpg	606.27	J/mol×K	826.58	Joback Method
cpg	615.02	J/mol×K	859.49	Joback Method
cpg	622.90	J/mol×K	892.39	Joback Method
cpg	629.91	J/mol×K	925.30	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=U374743&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