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

Inchi: InChI=1S/C14H12F7NO5S/c1-7-3-5-9(6-4-7)28(25,26)22-10(23)8(2)27-11(24)12(15,16)1

InchiKey: CKSMFGOGBNPQSD-UHFFFAOYSA-N

Formula: C14H12F7NO5S

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

Mol. weight [g/mol]: 439.30

Physical Properties

Property code	Value	Unit	Source
gf	-1929.80	kJ/mol	Joback Method
hf	-2268.79	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	80.67	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.565		Crippen Method
mcvol	243.830	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	764.25	K	Joback Method
tc	951.30	K	Joback Method
tf	496.18	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.62	J/mol×K	764.25	Joback Method
cpg	727.43	J/mol×K	795.43	Joback Method
cpg	737.29	J/mol×K	826.60	Joback Method
cpg	746.25	J/mol×K	857.78	Joback Method
cpg	754.36	J/mol×K	888.95	Joback Method
cpg	761.68	J/mol×K	920.13	Joback Method
cpg	768.24	J/mol×K	951.30	Joback Method

Sources

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=U374249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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