Benzoic acid, 4-methylsulfonylamino-

Inchi: InChI=1S/C8H9NO4S/c1-14(12,13)9-7-4-2-6(3-5-7)8(10)11/h2-5,9H,1H3,(H,10,11)
InchiKey: SROHFTOYGFCJAF-UHFFFAOYSA-N
Formula: C8H9NO4S
SMILES: CS(=O)(=O)Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 215.23
CAS: 7151-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-525.63	kJ/mol	Joback Method
hf	-648.08	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.756		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
tb	658.10	K	Joback Method
tc	858.88	K	Joback Method
tf	420.83	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.43	J/mol×K	658.10	Joback Method
cpg	367.01	J/mol×K	691.56	Joback Method
cpg	375.90	J/mol×K	725.03	Joback Method
cpg	384.13	J/mol×K	758.49	Joback Method
cpg	391.69	J/mol×K	791.96	Joback Method
cpg	398.60	J/mol×K	825.42	Joback Method
cpg	404.86	J/mol×K	858.88	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=C7151760&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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