3-Sulfamylbenzoic acid

Inchi: InChI=1S/C7H7NO4S/c8-13(11,12)6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)(H2,8,11,12)
InchiKey: NAETXYOXMDYNLE-UHFFFAOYSA-N
Formula: C7H7NO4S
SMILES: NS(=O)(=O)c1cccc(C(=O)O)c1
Mol. weight [g/mol]: 201.20
CAS: 636-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-556.99	kJ/mol	Joback Method
hf	-647.12	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.032		Crippen Method
mcvol	131.240	ml/mol	McGowan Method
pc	6864.13	kPa	Joback Method
tb	657.58	K	Joback Method
tc	868.47	K	Joback Method
tf	440.16	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.53	J/mol×K	657.58	Joback Method
cpg	325.02	J/mol×K	692.73	Joback Method
cpg	332.85	J/mol×K	727.88	Joback Method
cpg	340.02	J/mol×K	763.02	Joback Method
cpg	346.55	J/mol×K	798.17	Joback Method
cpg	352.44	J/mol×K	833.32	Joback Method
cpg	357.69	J/mol×K	868.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C636760&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume