

Acetic acid, sulfonyldi-

Inchi:	InChI=1S/C4H6O6S/c5-3(6)1-11(9,10)2-4(7)8/h1-2H2,(H,5,6)(H,7,8)
InchiKey:	WDYRPTWUNMHTJL-UHFFFAOYSA-N
Formula:	C4H6O6S
SMILES:	O=C(O)CS(=O)(=O)CC(=O)O
Mol. weight [g/mol]:	182.15
CAS:	123-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-1017.22	kJ/mol	Joback Method
hf	-1108.86	kJ/mol	Joback Method
hfus	28.87	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	1.47		Crippen Method
logp	-1.430		Crippen Method
mcvol	110.190	ml/mol	McGowan Method
pc	7735.33	kPa	Joback Method
tb	630.80	K	Joback Method
tc	804.18	K	Joback Method
tf	394.90	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.98	J/molxK	630.80	Joback Method
cpg	267.82	J/molxK	659.70	Joback Method
cpg	273.33	J/molxK	688.59	Joback Method
cpg	278.49	J/molxK	717.49	Joback Method
cpg	283.32	J/molxK	746.38	Joback Method
cpg	287.79	J/molxK	775.28	Joback Method
cpg	291.91	J/molxK	804.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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