4-Acetamidothioan1sole

Other names: 4'-(Methylthio)acetanilide
4-Acetamidothioanisole
Inchi: InChI=1S/C9H11NOS/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)
InchiKey: IYTZTJQAOQJQGD-UHFFFAOYSA-N
Formula: C9H11NOS
SMILES: CSc1ccc(NC(C)=O)cc1
Mol. weight [g/mol]: 181.25
CAS: 10352-44-0

Physical Properties

Property code	Value	Unit	Source
gf	121.27	kJ/mol	Joback Method
hf	-21.27	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	58.56	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.367		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	609.80	K	Joback Method
tc	848.68	K	Joback Method
tf	367.12	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.05	J/mol×K	609.80	Joback Method
cpg	338.72	J/mol×K	649.61	Joback Method
cpg	350.49	J/mol×K	689.43	Joback Method
cpg	361.40	J/mol×K	729.24	Joback Method
cpg	371.46	J/mol×K	769.06	Joback Method
cpg	380.71	J/mol×K	808.87	Joback Method
cpg	389.16	J/mol×K	848.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10352440&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