4-Acetamidothioanisole

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]: 181.26

Physical Properties

Property code	Value	Unit	Source
hfus	23.55	kJ/mol	Joback Method
ie	7.69	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	2.367		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
tb	588.86	K	Cheméo Relay (1.0)
tf	370.90	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10352440&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point