3-Aminothiophenol, N,S-diacetyl-

Inchi: InChI=1S/C10H11NO2S/c1-7(12)11-9-4-3-5-10(6-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)
InchiKey: WYTMCCIDRRAWCD-UHFFFAOYSA-N
Formula: C10H11NO2S
SMILES: CC(=O)Nc1cccc(SC(C)=O)c1
Mol. weight [g/mol]: 209.26

Physical Properties

Property code	Value	Unit	Source
gf	0.77	kJ/mol	Joback Method
hf	-154.49	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	67.54	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.284		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	2019.10		NIST Webbook
tb	686.55	K	Joback Method
tc	926.64	K	Joback Method
tf	428.32	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.22	J/mol×K	686.55	Joback Method
cpg	398.07	J/mol×K	726.56	Joback Method
cpg	408.98	J/mol×K	766.58	Joback Method
cpg	418.97	J/mol×K	806.59	Joback Method
cpg	428.06	J/mol×K	846.61	Joback Method
cpg	436.30	J/mol×K	886.62	Joback Method
cpg	443.70	J/mol×K	926.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353078&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume