3-Aminothiophenol, N,N,S-trimethyl-

Inchi: InChI=1S/C9H13NS/c1-10(2)8-5-4-6-9(7-8)11-3/h4-7H,1-3H3
InchiKey: OTIDSYZPXOTMOC-UHFFFAOYSA-N
Formula: C9H13NS
SMILES: CSc1cccc(N(C)C)c1
Mol. weight [g/mol]: 167.27

Physical Properties

Property code	Value	Unit	Source
gf	271.58	kJ/mol	Joback Method
hf	105.37	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	47.43	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.475		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1554.20		NIST Webbook
tb	518.20	K	Joback Method
tc	746.36	K	Joback Method
tf	297.00	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.54	J/mol×K	518.20	Joback Method
cpg	313.41	J/mol×K	556.23	Joback Method
cpg	327.35	J/mol×K	594.25	Joback Method
cpg	340.37	J/mol×K	632.28	Joback Method
cpg	352.53	J/mol×K	670.30	Joback Method
cpg	363.85	J/mol×K	708.33	Joback Method
cpg	374.37	J/mol×K	746.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353081&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
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
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