3,5-Dimethylthiophenol, S-methyl-

Inchi: InChI=1S/C9H12S/c1-7-4-8(2)6-9(5-7)10-3/h4-6H,1-3H3
InchiKey: ZHRCEGLNBBUOOS-UHFFFAOYSA-N
Formula: C9H12S
SMILES: CSc1cc(C)cc(C)c1
Mol. weight [g/mol]: 152.26

Physical Properties

Property code	Value	Unit	Source
gf	151.17	kJ/mol	Joback Method
hf	26.37	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.025		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1313.30		NIST Webbook
rinpol	1313.30		NIST Webbook
tb	510.74	K	Joback Method
tc	743.84	K	Joback Method
tf	277.05	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.39	J/mol×K	510.74	Joback Method
cpg	279.00	J/mol×K	549.59	Joback Method
cpg	291.85	J/mol×K	588.44	Joback Method
cpg	303.97	J/mol×K	627.29	Joback Method
cpg	315.36	J/mol×K	666.14	Joback Method
cpg	326.04	J/mol×K	704.99	Joback Method
cpg	336.02	J/mol×K	743.84	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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