4-Isopropylthiophenol

Other names: 4-Isopropylbenzenethiol
Inchi: InChI=1S/C9H12S/c1-7(2)8-3-5-9(10)6-4-8/h3-7,10H,1-2H3
InchiKey: APDUDRFJNCIWAG-UHFFFAOYSA-N
Formula: C9H12S
SMILES: CC(C)c1ccc(S)cc1
Mol. weight [g/mol]: 152.26
CAS: 4946-14-9

Physical Properties

Property code	Value	Unit	Source
gf	154.63	kJ/mol	Joback Method
hf	29.17	kJ/mol	Joback Method
hfus	13.24	kJ/mol	Joback Method
hvap	44.92	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.099		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1192.00		NIST Webbook
rinpol	1258.70		NIST Webbook
rinpol	1192.00		NIST Webbook
tb	499.40	K	Joback Method
tc	737.25	K	Joback Method
tf	251.59	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.72	J/mol×K	499.40	Joback Method
cpg	278.10	J/mol×K	539.04	Joback Method
cpg	291.56	J/mol×K	578.68	Joback Method
cpg	304.15	J/mol×K	618.33	Joback Method
cpg	315.90	J/mol×K	657.97	Joback Method

cpg	326.85	J/mol×K	697.61	Joback Method
cpg	337.03	J/mol×K	737.25	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=C4946149&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