2-Isopropylbenzenethiol, S-acetyl-

Inchi: InChI=1S/C11H14OS/c1-8(2)10-6-4-5-7-11(10)13-9(3)12/h4-8H,1-3H3
InchiKey: MJJNVMKMEPMOKV-UHFFFAOYSA-N
Formula: C11H14OS
SMILES: CC(=O)Sc1ccccc1C(C)C
Mol. weight [g/mol]: 194.29

Physical Properties

Property code	Value	Unit	Source
gf	46.28	kJ/mol	Joback Method
hf	-121.30	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.449		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1452.50		NIST Webbook
tb	604.95	K	Joback Method
tc	841.20	K	Joback Method
tf	322.00	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.21	J/mol×K	604.95	Joback Method
cpg	389.04	J/mol×K	644.33	Joback Method
cpg	402.87	J/mol×K	683.70	Joback Method
cpg	415.73	J/mol×K	723.08	Joback Method
cpg	427.66	J/mol×K	762.45	Joback Method
cpg	438.67	J/mol×K	801.83	Joback Method
cpg	448.81	J/mol×K	841.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353042&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