Phenol, 3,5-dimethyl-4-(methylthio)-

Other names: 4-(methylthio)-3,5-xylenol
Inchi: InChI=1S/C9H12OS/c1-6-4-8(10)5-7(2)9(6)11-3/h4-5,10H,1-3H3
InchiKey: JGFZITGNFAVSKU-UHFFFAOYSA-N
Formula: C9H12OS
SMILES: CSc1c(C)cc(O)cc1C
Mol. weight [g/mol]: 168.26
CAS: 7379-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-3.45	kJ/mol	Joback Method
hf	-150.94	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.731		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1530.00		NIST Webbook
tb	591.36	K	Joback Method
tc	835.91	K	Joback Method
tf	388.77	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.17	J/mol×K	591.36	Joback Method
cpg	325.41	J/mol×K	632.12	Joback Method
cpg	336.84	J/mol×K	672.88	Joback Method
cpg	347.54	J/mol×K	713.64	Joback Method
cpg	357.58	J/mol×K	754.39	Joback Method
cpg	367.02	J/mol×K	795.15	Joback Method
cpg	375.94	J/mol×K	835.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7379513&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