

2,6-Dimethylbenzenethiol, S-methyl-

Inchi:	InChI=1S/C9H12S/c1-7-5-4-6-8(2)9(7)10-3/h4-6H,1-3H3
InchiKey:	ITVXUDPAZIIKED-UHFFFAOYSA-N
Formula:	C9H12S
SMILES:	CSc1c(C)cccc1C
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	1256.00		NIST Webbook
rinpol	1259.30		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1259.30		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/molxK	510.74	Joback Method
cpg	279.00	J/molxK	549.59	Joback Method
cpg	291.85	J/molxK	588.44	Joback Method
cpg	303.97	J/molxK	627.29	Joback Method
cpg	315.36	J/molxK	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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