2,6-Dimethylthiophenol

Other names:	2,6-Dimethylbenzenethiol
	Benzenethiol, 2,6-dimethyl-
Inchi:	InChI=1S/C8H10S/c1-6-4-3-5-7(2)8(6)9/h3-5,9H,1-2H3
InchiKey:	QCLJODDRBGKIRW-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	Cc1cccc(C)c1S
Mol. weight [g/mol]:	138.23
CAS:	118-72-9

Physical Properties

Property code	Value	Unit	Source
gf	139.02	kJ/mol	Joback Method
hf	43.62	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	43.74	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.592		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1213.20		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	481.94	K	Joback Method
tc	719.76	K	Joback Method
tf	267.84	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.55	J/mol×K	481.94	Joback Method
cpg	233.86	J/mol×K	521.58	Joback Method
cpg	245.45	J/mol×K	561.21	Joback Method
cpg	256.34	J/mol×K	600.85	Joback Method

cpg	266.57	J/mol×K	640.49	Joback Method
cpg	276.15	J/mol×K	680.13	Joback Method
cpg	285.11	J/mol×K	719.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47964e+01
Coeff. B	-4.16901e+03
Coeff. C	-7.72170e+01
Temperature range (K), min.	364.56
Temperature range (K), max.	516.76

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118729&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

pvap:	Vapor 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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