2,5-DIMETHYLTHIOPHENOL

Other names: 2,5-Dimethylbenzenethiol
Benzenethiol, 2,5-dimethyl-
Inchi: InChI=1S/C8H10S/c1-6-3-4-7(2)8(9)5-6/h3-5,9H,1-2H3
InchiKey: NHAUBUMQRJWWAT-UHFFFAOYSA-N
Formula: C8H10S
SMILES: Cc1ccc(C)c(S)c1
Mol. weight [g/mol]: 138.24
CAS: 4001-61-0

Physical Properties

Property code	Value	Unit	Source
af	0.3694		Cheméo Relay (1.0)
gf	139.02	kJ/mol	Joback Method
hf	48.52	kJ/mol	Cheméo Relay (1.0)
hfus	13.78	kJ/mol	Joback Method
hvap	56.39	kJ/mol	Cheméo Relay (1.0)
ie	7.94	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.592		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1206.20		NIST Webbook
rinpol	1206.20		NIST Webbook
tb	485.25	K	Cheméo Relay (1.0)
tc	706.42	K	Cheméo Relay (1.0)
tf	305.23	K	Cheméo Relay (1.0)
vc	0.412	m3/kmol	Cheméo Relay (1.0)

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.50	K	6.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39532e+01
Coeff. B	-3.85293e+03
Coeff. C	-7.40760e+01
Temperature range (K), min.	356.02
Temperature range (K), max.	519.93

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4001610&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume