

Thiophene, 2,4-dimethyl-

Other names:	2,4-Dimethylthiophene
Inchi:	InChI=1S/C6H8S/c1-5-3-6(2)7-4-5/h3-4H,1-2H3
InchiKey:	CPULIKNSOUFMPL-UHFFFAOYSA-N
Formula:	C6H8S
SMILES:	Cc1csc(C)c1
Mol. weight [g/mol]:	112.19
CAS:	638-00-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	2.365		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
rinpol	860.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	855.80		NIST Webbook
rinpol	882.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1231.00		NIST Webbook

ripol	1190.00	NIST Webbook
ripol	1181.00	NIST Webbook
ripol	1197.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1253.00	NIST Webbook
ripol	1244.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	41.40	kJ/mol	408.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47364e+01
Coeff. B	-3.51538e+03
Coeff. C	-6.08830e+01
Temperature range (K), min.	304.18
Temperature range (K), max.	433.87

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1883.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638006&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/47-133-2/Thiophene-2-4-dimethyl.pdf>

Generated by Cheméo on 2024-04-27 10:04:20.315278814 +0000 UTC m=+16501509.235856129.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.