

Thiophene, 2-pentyl-

Other names:	1-methylbutylthiophene 2-Pentylthiophene 2-n-Amylthiophene 2-n-Pentylthiophene
Inchi:	InChI=1S/C9H14S/c1-2-3-4-6-9-7-5-8-10-9/h5,7-8H,2-4,6H2,1H3
InchiKey:	NOYVOSGVFSEKPR-UHFFFAOYSA-N
Formula:	C9H14S
SMILES:	CCCCC1cccs1
Mol. weight [g/mol]:	154.27
CAS:	4861-58-9

Physical Properties

Property code	Value	Unit	Source
hvap	52.00 ± 1.20	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	3.481		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1452.00		NIST Webbook

ripol	1437.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1462.00	NIST Webbook
ripol	1456.00	NIST Webbook
ripol	1462.00	NIST Webbook
ripol	1438.00	NIST Webbook
ripol	1440.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50163e+01
Coeff. B	-4.17668e+03
Coeff. C	-7.41450e+01
Temperature range (K), min.	357.72
Temperature range (K), max.	504.52

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4861589&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
pvap:	Vapor pressure
ripol:	Non-polar retention indices

ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/67-863-0/Thiophene-2-pentyl.pdf>

Generated by Cheméo on 2024-04-25 04:04:07.559455925 +0000 UTC m=+16307096.480033236.

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