

Thiophane, 3-pentyl-

Other names:	3-Pentyltetrahydrothiophene Thiolane, 3-pentyl 3-Amylthiophane 3-Pentylthiophane Thiophene, tetrahydro-3-pentyl- Thiolane, 2-pentyl
Inchi:	InChI=1S/C9H18S/c1-2-3-4-5-9-6-7-10-8-9/h9H,2-8H2,1H3
InchiKey:	PTJARFWPUNOHQM-UHFFFAOYSA-N
Formula:	C9H18S
SMILES:	CCCCC1CCSC1
Mol. weight [g/mol]:	158.30
CAS:	35468-43-0

Physical Properties

Property code	Value	Unit	Source
gf	101.31	kJ/mol	Joback Method
hf	-123.35	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.320		Crippen Method
mvol	143.160	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	468.43	K	Joback Method
tc	673.79	K	Joback Method
tf	285.54	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.34	J/mol×K	468.43	Joback Method

cpg	324.89	J/mol×K	502.66	Joback Method
cpg	341.51	J/mol×K	536.88	Joback Method
cpg	357.25	J/mol×K	571.11	Joback Method
cpg	372.13	J/mol×K	605.34	Joback Method
cpg	386.19	J/mol×K	639.56	Joback Method
cpg	399.47	J/mol×K	673.79	Joback Method

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=C35468430&Units=SI
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
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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