1-Pentanethiol

Other names:	1-Mercaptopentane
	1-Pentanthiol
	1-Pentylthiol
	Amyl hydrosulfide
	Amyl mercaptan
	Amyl sulfhydrate
	Amyl thioalcohol
	CH3(CH2)4SH
	Mercaptan amylique
	Pentalarm
	Pentane-1-thiol
	Pentanethiol
	Pentyl mercaptan
	n-Amyl mercaptan
	n-Pentyl mercaptan
Inchi:	InChI=1S/C5H12S/c1-2-3-4-5-6/h6H,2-5H2,1H3
InchiKey:	ZRKMQKLGEQPLNS-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCCCCS
Mol. weight [g/mol]:	104.21
CAS:	110-66-7

Physical Properties

Property code	Value	Unit	Source
chl	-4132.60 ± 1.50	kJ/mol	NIST Webbook
chl	-4133.80	kJ/mol	NIST Webbook
chl	-4151.00	kJ/mol	NIST Webbook
gf	20.61	kJ/mol	Joback Method
hf	-109.70	kJ/mol	NIST Webbook
hf	-110.80 ± 1.80	kJ/mol	NIST Webbook
hfl	-150.90 ± 0.84	kJ/mol	NIST Webbook
hfl	-152.00 ± 1.70	kJ/mol	NIST Webbook
hfus	12.75	kJ/mol	Joback Method
hvap	41.20	kJ/mol	NIST Webbook
hvap	41.10	kJ/mol	NIST Webbook
hvap	41.10	kJ/mol	NIST Webbook
hvap	41.26	kJ/mol	NIST Webbook

log10ws	-1.99		Crippen Method
logp	2.106		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	803.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	818.90		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	828.80		NIST Webbook
rinpol	821.70		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	821.10		NIST Webbook
ripol	1039.00		NIST Webbook
ripol	1047.90		NIST Webbook
ripol	1052.90		NIST Webbook
ripol	1063.00		NIST Webbook
sl	310.37	J/mol×K	NIST Webbook
tb	399.80	K	NIST Webbook
tb	398.00 ± 1.00	K	NIST Webbook
tb	397.00 ± 2.50	K	NIST Webbook
tb	399.20	K	NIST Webbook
tb	399.00	K	NIST Webbook
tc	597.70	K	NIST Webbook
tf	197.50 ± 0.30	K	NIST Webbook
tf	197.50 ± 0.50	K	NIST Webbook
tt	197.46 ± 0.02	K	NIST Webbook
tt	197.45 ± 0.02	K	NIST Webbook
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.90	J/mol×K	566.46	Joback Method
cpg	178.44	J/mol×K	408.29	Joback Method
cpg	188.11	J/mol×K	439.93	Joback Method
cpg	197.38	J/mol×K	471.56	Joback Method
cpg	206.26	J/mol×K	503.19	Joback Method
cpg	214.76	J/mol×K	534.82	Joback Method
cpg	168.36	J/mol×K	376.66	Joback Method
cpl	201.17	J/mol×K	296.21	NIST Webbook
hfust	17.53	kJ/mol	197.50	NIST Webbook
hfust	17.53	kJ/mol	197.46	NIST Webbook
hfust	17.53	kJ/mol	197.50	NIST Webbook
hvapt	34.88	kJ/mol	399.80	NIST Webbook
hvapt	40.60	kJ/mol	363.00	NIST Webbook
hvapt	38.10	kJ/mol	393.50	NIST Webbook
hvapt	37.10 ± 0.10	kJ/mol	356.00	NIST Webbook
hvapt	36.40 ± 0.10	kJ/mol	376.00	NIST Webbook
hvapt	34.90 ± 0.10	kJ/mol	400.00	NIST Webbook
sfust	88.78	J/mol×K	197.46	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54679e+01
Coeff. B	-3.76382e+03
Coeff. C	-5.22920e+01
Temperature range (K), min.	300.23
Temperature range (K), max.	422.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.71980e+01

Coeff. B	-7.40124e+03
Coeff. C	-9.16808e+00
Coeff. D	5.36099e-06
Temperature range (K), min.	197.45
Temperature range (K), max.	598.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110667&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1827
An improved static-analytic apparatus for vapor-liquid equilibrium (PTxy) measurement using modified in-situ samplers:	https://www.doi.org/10.1016/j.fluid.2015.10.041
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1819.mol

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature

sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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