

1,5-Pentanedithiol

Other names:	1,5-Dimercaptopentane pentane-1,5-dithiol
Inchi:	InChI=1S/C5H12S2/c6-4-2-1-3-5-7/h6-7H,1-5H2
InchiKey:	KMTUBAIXCBHPIZ-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	SCCCCCS
Mol. weight [g/mol]:	136.28
CAS:	928-98-3

Physical Properties

Property code	Value	Unit	Source
chl	-4757.10 ± 1.20	kJ/mol	NIST Webbook
gf	50.00	kJ/mol	Joback Method
hf	-71.00 ± 1.50	kJ/mol	NIST Webbook
hfl	-130.30 ± 1.30	kJ/mol	NIST Webbook
hfus	16.79	kJ/mol	Joback Method
hvap	59.30	kJ/mol	NIST Webbook
hvap	59.30	kJ/mol	NIST Webbook
hvap	59.29 ± 0.42	kJ/mol	NIST Webbook
hvap	59.29	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.016		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1672.00		NIST Webbook
tb	439.52	K	Joback Method
tc	654.99	K	Joback Method
tf	219.03	K	Joback Method
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.16	J/mol×K	619.08	Joback Method
cpg	211.02	J/mol×K	439.52	Joback Method
cpg	221.89	J/mol×K	475.43	Joback Method
cpg	232.22	J/mol×K	511.34	Joback Method
cpg	242.03	J/mol×K	547.25	Joback Method
cpg	251.34	J/mol×K	583.17	Joback Method
cpg	268.52	J/mol×K	654.99	Joback Method
hvapt	51.60	kJ/mol	427.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52519e+01
Coeff. B	-4.82198e+03
Coeff. C	-4.03040e+01
Temperature range (K), min.	362.54
Temperature range (K), max.	525.39

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=C928983&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
rinpola:	Non-polar retention indices
ripola:	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

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