1,3-Propanedithiol

Other names:	1,3-Dimercaptopropane
	1,3-Propanedimercaptan
	Dithiotrimethyleneglycol
	NDR-132
	Trimethylene dimercaptan
	Trimethylenedithioglycol
	Trimethylenedithiol
	propane-1,3-dithiol
Inchi:	InChI=1S/C3H8S2/c4-2-1-3-5/h4-5H,1-3H2
InchiKey:	ZJLMKPKYJBQJNH-UHFFFAOYSA-N
Formula:	C3H8S2
SMILES:	SCCCS
Mol. weight [g/mol]:	108.23
CAS:	109-80-8

Physical Properties

Property code	Value	Unit	Source
chl	-3449.20 ± 1.10	kJ/mol	NIST Webbook
gf	33.16	kJ/mol	Joback Method
hf	-29.80 ± 1.20	kJ/mol	NIST Webbook
hfl	-79.50 ± 1.20	kJ/mol	NIST Webbook
hfus	11.61	kJ/mol	Joback Method
hvap	49.70	kJ/mol	NIST Webbook
hvap	49.70	kJ/mol	NIST Webbook
hvap	49.70 ± 0.10	kJ/mol	NIST Webbook
hvap	49.66	kJ/mol	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.236		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	921.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1457.00		NIST Webbook

ripol	1448.00		NIST Webbook
tb	442.20	K	NIST Webbook
tc	614.54	K	Joback Method
tf	196.49	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.78	J/mol×K	393.76	Joback Method
cpg	146.50	J/mol×K	430.56	Joback Method
cpg	153.84	J/mol×K	467.35	Joback Method
cpg	160.82	J/mol×K	504.15	Joback Method
cpg	167.45	J/mol×K	540.94	Joback Method
cpg	173.74	J/mol×K	577.74	Joback Method
cpg	179.70	J/mol×K	614.54	Joback Method
hvapt	50.90	kJ/mol	392.00	NIST Webbook
hvapt	41.60	kJ/mol	411.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61058e+01
Coeff. B	-5.08533e+03
Coeff. C	4.84000e-01
Temperature range (K), min.	321.00
Temperature range (K), max.	473.19

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109808&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume