1,2-Propanedithiol

Other names:	1,2-Dimercaptopropane
	1,2-Dithiolpropane
	1,2-Propanedithiol-propylene dimercaptan
	2,3-Dimercaptopropane
	propane-1,2-dithiol
Inchi:	InChI=1S/C3H8S2/c1-3(5)2-4/h3-5H,2H2,1H3
InchiKey:	YGKHJWTVMIMEPQ-UHFFFAOYSA-N
Formula:	C3H8S2
SMILES:	CC(S)CS
Mol. weight [g/mol]:	108.23
CAS:	814-67-5

Physical Properties

Property code	Value	Unit	Source
gf	30.72	kJ/mol	Joback Method
hf	-33.57	kJ/mol	Joback Method
hfus	8.09	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.235		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	880.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook
tb	393.32	K	Joback Method
tc	619.83	K	Joback Method
tf	181.49	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.81	J/mol×K	393.32	Joback Method
cpg	146.84	J/mol×K	431.07	Joback Method
cpg	154.47	J/mol×K	468.82	Joback Method
cpg	161.70	J/mol×K	506.57	Joback Method
cpg	168.56	J/mol×K	544.33	Joback Method
cpg	175.04	J/mol×K	582.08	Joback Method
cpg	181.16	J/mol×K	619.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28839e+01
Coeff. B	-3.19667e+03
Coeff. C	-5.93420e+01
Temperature range (K), min.	313.12
Temperature range (K), max.	481.49

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=C814675&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

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
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