1,6-Hexanedithiol

Other names:	1,6-Dimercaptohexane
	1,6-Hexanedimercaptan
	Hexanedithiol-(1,6)
	NDR-139
	USAF uctl-72
	hexane-1,6-dithiol
Inchi:	InChI=1S/C6H14S2/c7-5-3-1-2-4-6-8/h7-8H,1-6H2
InchiKey:	SRZXCOWFGPICGA-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	SCCCCCCS
Mol. weight [g/mol]:	150.31
CAS:	1191-43-1

Physical Properties

Property code	Value	Unit	Source
gf	58.42	kJ/mol	Joback Method
hf	-90.21	kJ/mol	Joback Method
hfus	19.38	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.406		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1255.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1770.00		NIST Webbook
tb	462.40	K	Joback Method
tc	674.93	K	Joback Method
tf	230.30	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.57	J/mol×K	462.40	Joback Method
cpg	262.76	J/mol×K	497.82	Joback Method
cpg	274.35	J/mol×K	533.24	Joback Method
cpg	285.35	J/mol×K	568.66	Joback Method
cpg	295.79	J/mol×K	604.09	Joback Method
cpg	305.68	J/mol×K	639.51	Joback Method
cpg	315.04	J/mol×K	674.93	Joback Method
hvapt	55.70	kJ/mol	445.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43816e+01
Coeff. B	-4.23707e+03
Coeff. C	-8.10830e+01
Temperature range (K), min.	379.00
Temperature range (K), max.	548.23

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191431&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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume