Cyclohexanethiol

Other names:	CYCLOHEXYL MERCAPTAN
	CYCLOHEXYL THIOL
	Cyklohexanthiol
	Cyklohexylmerkaptan
Inchi:	InChI=1S/C6H12S/c7-6-4-2-1-3-5-6/h6-7H,1-5H2
InchiKey:	CMKBCTPCXZNQKX-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	SC1CCCCC1
Mol. weight [g/mol]:	116.22
CAS:	1569-69-3

Physical Properties

Property code	Value	Unit	Source
af	0.2520		KDB
chl	-4537.60 ± 3.60	kJ/mol	NIST Webbook
gf	53.48	kJ/mol	Joback Method
hf	-95.73 ± 0.79	kJ/mol	NIST Webbook
hf	-95.69	kJ/mol	NIST Webbook
hfl	-140.40 ± 0.79	kJ/mol	NIST Webbook
hfus	7.17	kJ/mol	Joback Method
hvap	44.90	kJ/mol	NIST Webbook
hvap	44.70	kJ/mol	NIST Webbook
hvap	44.60 ± 0.20	kJ/mol	NIST Webbook
hvap	44.60 ± 0.10	kJ/mol	NIST Webbook
hvap	44.57	kJ/mol	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.249		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3850.00	kPa	KDB
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
sl	255.57	J/mol×K	NIST Webbook
tb	431.98	K	KDB
tb	432.00	K	NIST Webbook
tb	431.95 ± 0.20	K	NIST Webbook
tb	427.00 ± 4.00	K	NIST Webbook

tb	428.00 ± 3.00	K	NIST Webbook
tb	432.20	K	NIST Webbook
tc	664.00	K	NIST Webbook
tc	664.20	K	KDB
tf	201.22	K	Joback Method
tt	189.63 ± 0.01	K	NIST Webbook
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.05	J/mol×K	419.09	Joback Method
cpg	266.56	J/mol×K	652.03	Joback Method
cpg	254.91	J/mol×K	613.20	Joback Method
cpg	242.46	J/mol×K	574.38	Joback Method
cpg	229.17	J/mol×K	535.56	Joback Method
cpg	215.02	J/mol×K	496.74	Joback Method
cpg	199.99	J/mol×K	457.91	Joback Method
cpl	192.63	J/mol×K	298.15	NIST Webbook
hfust	10.00	kJ/mol	189.64	NIST Webbook
hfust	10.00	kJ/mol	189.60	NIST Webbook
hfust	10.00	kJ/mol	189.60	NIST Webbook
hvapt	41.20	kJ/mol	415.50	NIST Webbook
hvapt	37.06	kJ/mol	432.00	NIST Webbook
rhol	964.63	kg/m3	293.10	KDB
sfust	52.73	J/mol×K	189.64	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38045e+01
Coeff. B	-3.38746e+03
Coeff. C	-6.34450e+01
Temperature range (K), min.	314.05
Temperature range (K), max.	462.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.04880e+01
Coeff. B	-7.97423e+03
Coeff. C	-9.62230e+00
Coeff. D	5.26186e-06
Temperature range (K), min.	355.15
Temperature range (K), max.	476.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1569693&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1886
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1886.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
rhol:	Liquid Density
rinpol:	Non-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