

Cyclopentanethiol

Other names:	CYCLOPENTYL MERCAPTANE Cyclopentyl mercaptan MERCAPTOCYCLOPENTANE
Inchi:	InChI=1S/C5H10S/c6-5-3-1-2-4-5/h5-6H,1-4H2
InchiKey:	WVDYBOADDMMFIY-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	SC1CCCC1
Mol. weight [g/mol]:	102.20
CAS:	1679-07-8

Physical Properties

Property code	Value	Unit	Source
af	0.2530		KDB
chl	-3909.50 ± 0.63	kJ/mol	NIST Webbook
gf	57.16	kJ/mol	Joback Method
hf	-47.78 ± 0.75	kJ/mol	NIST Webbook
hfl	-89.33 ± 0.75	kJ/mol	NIST Webbook
hfus	6.68	kJ/mol	Joback Method
hvap	41.50	kJ/mol	NIST Webbook
hvap	41.60	kJ/mol	NIST Webbook
hvap	41.44	kJ/mol	NIST Webbook
log10ws	-1.99		Crippen Method
logp	1.859		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	4275.00	kPa	KDB
rinpol	829.00		NIST Webbook
rinpol	829.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1111.00		NIST Webbook
sl	256.86	J/molxK	NIST Webbook
tb	405.30	K	KDB
tb	405.33	K	NIST Webbook
tb	405.35 ± 0.20	K	NIST Webbook
tb	404.70	K	NIST Webbook
tc	633.50	K	NIST Webbook
tc	629.00	K	KDB

tf	155.40	K	KDB
tt	155.39 ± 0.06	K	NIST Webbook
vc	0.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.70	J/mol×K	429.60	Joback Method
cpg	173.40	J/mol×K	467.26	Joback Method
cpg	147.21	J/mol×K	391.94	Joback Method
cpg	216.93	J/mol×K	617.90	Joback Method
cpg	207.08	J/mol×K	580.24	Joback Method
cpg	196.56	J/mol×K	542.58	Joback Method
cpg	185.34	J/mol×K	504.92	Joback Method
cpl	265.23	J/mol×K	298.15	NIST Webbook
hfust	7.83	kJ/mol	155.40	NIST Webbook
hfust	7.83	kJ/mol	155.40	NIST Webbook
hvapt	35.32	kJ/mol	405.33	NIST Webbook
hvapt	35.30 ± 0.10	kJ/mol	405.00	NIST Webbook
hvapt	36.70 ± 0.10	kJ/mol	381.00	NIST Webbook
hvapt	37.90 ± 0.10	kJ/mol	361.00	NIST Webbook
hvapt	38.40	kJ/mol	397.00	NIST Webbook
hvapt	38.20	kJ/mol	400.00	NIST Webbook
hvapt	35.33	kJ/mol	405.30	KDB
rhoI	960.62	kg/m ³	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	99.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43087e+01
Coeff. B	-3.40849e+03
Coeff. C	-5.29590e+01
Temperature range (K), min.	291.15
Temperature range (K), max.	431.80

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.49134e+01
Coeff. B	-7.32100e+03
Coeff. C	-8.84182e+00
Coeff. D	5.23512e-06
Temperature range (K), min.	348.15
Temperature range (K), max.	629.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1877.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679078&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1877

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
rho:	Liquid Density
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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