Ethanethiol, 2-(dimethylamino)-

Other names:	2-(Dimethylamino)-1-ethanethiol
	2-(dimethylamino)ethane-1-thiol
	2-(dimethylamino)ethanethiol
	2-Dimethylaminoethanethiol
	N-Dimethyl cysteamin
	N-Dimethyl cysteamine
	captamine
Inchi:	InChI=1S/C4H11NS/c1-5(2)3-4-6/h6H,3-4H2,1-2H3
InchiKey:	DENMGZODXQRYAR-UHFFFAOYSA-N
Formula:	C4H11NS
SMILES:	CN(C)CCS
Mol. weight [g/mol]:	105.20
CAS:	108-02-1

Physical Properties

Property code	Value	Unit	Source
gf	122.97	kJ/mol	Joback Method
hf	-19.88	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	33.28	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	0.478		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	396.50 ± 3.50	K	NIST Webbook
tc	555.22	K	Joback Method
tf	203.77	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.20	J/mol×K	366.22	Joback Method
cpg	169.23	J/mol×K	397.72	Joback Method

cpg	178.81	J/mol×K	429.22	Joback Method
cpg	187.93	J/mol×K	460.72	Joback Method
cpg	196.62	J/mol×K	492.22	Joback Method
cpg	204.88	J/mol×K	523.72	Joback Method
cpg	212.75	J/mol×K	555.22	Joback Method
pvap	0.07	kPa	278.15	Vapor Pressure of 2-Dialkyl Aminoethanethiols
pvap	0.14	kPa	287.15	Vapor Pressure of 2-Dialkyl Aminoethanethiols
pvap	0.26	kPa	296.15	Vapor Pressure of 2-Dialkyl Aminoethanethiols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	319.00 ± 1.00	K	5.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapor Pressure of 2-Dialkyl Aminoethanethiols: https://www.doi.org/10.1021/je400136y

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=C108021&Units=SI

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