2-DIMETHYLAMINOETHANETHIOL

Other names:	2-(Dimethylamino)-1-ethanethiol
	2-(dimethylamino)ethane-1-thiol
	2-(dimethylamino)ethanethiol
	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]:	105.21

Physical Properties

Property code	Value	Unit	Source
hfus	13.18	kJ/mol	Joback Method
hvap	39.79	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
logp	0.478		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
tb	393.50	K	Cheméo Relay (1.0)
tf	163.33	K	Cheméo Relay (1.0)

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Vapor Pressure of 2-Dialkyl Aminoethanethiols:	https://www.doi.org/10.1021/je400136y
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108021&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point