N-Acetylcysteamine

Inchi: InChI=1S/C4H9NOS/c1-4(6)5-2-3-7/h7H,2-3H2,1H3,(H,5,6)
InchiKey: AXFZADXWLMXITO-UHFFFAOYSA-N
Formula: C4H9NOS
SMILES: CC(O)=NCCS
Mol. weight [g/mol]: 119.19
CAS: 20939-05-3

Physical Properties

Property code	Value	Unit	Source
hf	-167.21	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.893		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	522.52	K	Joback Method
tc	728.94	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20939053&Units=SI
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature