

2-(N'-Isopropylidenehydrazino)-ethanethiol

Inchi: InChI=1S/C5H12N2S/c1-5(2)7-6-3-4-8/h6,8H,3-4H2,1-2H3
InchiKey: DNRKZACXUZJRFF-UHFFFAOYSA-N
Formula: C5H12N2S
SMILES: CC(C)=NNCCS
Mol. weight [g/mol]: 132.23
CAS: 73418-91-4

Physical Properties

Property code	Value	Unit	Source
hf	17.85	kJ/mol	Joback Method
hvap	43.29	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	0.902		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	503.39	K	Joback Method
tc	722.63	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C73418914&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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