1,1-Ethanedithiol

Inchi: InChI=1S/C2H6S2/c1-2(3)4/h2-4H,1H3
InchiKey: DHBXNPKRAUYBTH-UHFFFAOYSA-N
Formula: C2H6S2
SMILES: CC(S)S
Mol. weight [g/mol]: 94.20

Physical Properties

Property code	Value	Unit	Source
gf	22.30	kJ/mol	Joback Method
hf	-12.93	kJ/mol	Joback Method
hfus	5.50	kJ/mol	Joback Method
hvap	33.13	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.192		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
rinpol	756.00		NIST Webbook
rinpol	756.00		NIST Webbook
tb	370.44	K	Joback Method
tc	599.35	K	Joback Method
tf	170.22	K	Joback Method
vc	0.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.31	J/mol×K	370.44	Joback Method
cpg	112.47	J/mol×K	408.59	Joback Method
cpg	118.32	J/mol×K	446.74	Joback Method
cpg	123.87	J/mol×K	484.90	Joback Method
cpg	129.14	J/mol×K	523.05	Joback Method
cpg	134.12	J/mol×K	561.20	Joback Method
cpg	138.84	J/mol×K	599.35	Joback Method

Sources

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=R61027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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