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
CAS: 69382-62-3

Physical Properties

Property code	Value	Unit	Source
af	0.3302		Cheméo Relay (1.0)
gf	22.30	kJ/mol	Joback Method
hf	-24.71	kJ/mol	Cheméo Relay (1.0)
hfus	5.50	kJ/mol	Joback Method
hvap	34.84	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-0.64		Cheméo Relay (1.0)
logp	1.192		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
tb	370.55	K	Cheméo Relay (1.0)
tc	603.78	K	Cheméo Relay (1.0)
tf	177.09	K	Cheméo Relay (1.0)
vc	0.259	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69382623&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume