2-HYDROXYETHYL VINYL SULFIDE

Other names: Ethanol, 2-(ethenylthio)-
Inchi: InChI=1S/C4H8OS/c1-2-6-4-3-5/h2,5H,1,3-4H2
InchiKey: CJDXLHTYSXHWDC-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: C=CSCCO
Mol. weight [g/mol]: 104.17

Physical Properties

Property code	Value	Unit	Source
hfus	13.05	kJ/mol	Joback Method
ie	8.63	eV	Cheméo Relay (1.0)
logp	0.855		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
rinpol	863.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	923.20		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	932.20		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	863.00		NIST Webbook
tb	455.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.69	J/mol×K	448.56	Joback Method
cpg	165.68	J/mol×K	479.86	Joback Method
cpg	172.37	J/mol×K	511.15	Joback Method
cpg	178.76	J/mol×K	542.45	Joback Method
cpg	184.86	J/mol×K	573.74	Joback Method
cpg	190.67	J/mol×K	605.04	Joback Method
cpg	196.21	J/mol×K	636.33	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3090560&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature