

Ethanol, 2-(methylthio)methylthio

Inchi:	InChI=1S/C4H10OS2/c1-6-4-7-3-2-5/h5H,2-4H2,1H3
InchiKey:	LEILLEQUGZHUJV-UHFFFAOYSA-N
Formula:	C4H10OS2
SMILES:	CSCSCCO
Mol. weight [g/mol]:	138.25

Physical Properties

Property code	Value	Unit	Source
gf	-87.78	kJ/mol	Joback Method
hf	-194.38	kJ/mol	Joback Method
hfus	18.46	kJ/mol	Joback Method
hvap	54.81	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.032		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
ripol	2090.00		NIST Webbook
ripol	2090.00		NIST Webbook
tb	520.66	K	Joback Method
tc	724.81	K	Joback Method
tf	264.46	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.19	J/molxK	520.66	Joback Method
cpg	223.50	J/molxK	554.69	Joback Method
cpg	231.44	J/molxK	588.71	Joback Method
cpg	239.01	J/molxK	622.74	Joback Method
cpg	246.21	J/molxK	656.76	Joback Method
cpg	253.03	J/molxK	690.79	Joback Method
cpg	259.48	J/molxK	724.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
ri pol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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