1-Propene-1-thiol

Other names: 1-Propenethiol
1-Propenylthiol
Inchi: InChI=1S/C3H6S/c1-2-3-4/h2-4H,1H3/b3-2+
InchiKey: RIZGKEIRSQLIBK-NSCUHMNNSA-N
Formula: C3H6S
SMILES: CC=CS
Mol. weight [g/mol]: 74.14
CAS: 925-89-3

Physical Properties

Property code	Value	Unit	Source
gf	83.99	kJ/mol	Joback Method
hf	50.45	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	28.97	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.450		Crippen Method
mcvol	65.180	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
rinpol	600.00		NIST Webbook
rinpol	603.40		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	600.00		NIST Webbook
tb	335.06	K	Joback Method
tc	537.26	K	Joback Method
tf	154.95	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.83	J/mol×K	335.06	Joback Method
cpg	95.31	J/mol×K	368.76	Joback Method
cpg	101.42	J/mol×K	402.46	Joback Method

cpg	107.18	J/mol×K	436.16	Joback Method
cpg	112.62	J/mol×K	469.86	Joback Method
cpg	117.75	J/mol×K	503.56	Joback Method
cpg	122.58	J/mol×K	537.26	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C925893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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