2-hydroxy-3-butenyl isothiocyanate

Inchi: InChI=1S/C6H9NS/c1-3-6(2)4-7-5-8/h3,6H,1,4H2,2H3
InchiKey: ISVIEXMVIMLCSG-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: C=CC(C)CN=C=S
Mol. weight [g/mol]: 127.21

Physical Properties

Property code	Value	Unit	Source
hf	237.05	kJ/mol	Joback Method
hvap	38.33	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.911		Crippen Method
mcvol	108.830	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1451.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	478.87	K	Joback Method
tc	703.48	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R512564&Units=SI

Legend

hf: Enthalpy of formation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature