Propargyl isothiocyanate

Other names: 2-Propynyl thiocyanate
Inchi: InChI=1S/C4H3NS/c1-2-3-5-4-6/h1H,3H2
InchiKey: XCXOHPXTLZMKQJ-UHFFFAOYSA-N
Formula: C4H3NS
SMILES: C#CCN=C=S
Mol. weight [g/mol]: 97.14

Physical Properties

Property code	Value	Unit	Source
hvap	46.92	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
logp	0.722		Crippen Method
mcvol	76.350	ml/mol	McGowan Method

Sources

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=C24309486&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume