

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

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