5-isothiocyano-1-pentene

Other names: 4-pentenyl isothiocyanate
Inchi: InChI=1S/C6H9NS/c1-2-3-4-5-7-6-8/h2H,1,3-5H2
InchiKey: DBISBKDNOKIADM-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: C=CCCCN=C=S
Mol. weight [g/mol]: 127.21

Physical Properties

Property code	Value	Unit	Source
hf	242.33	kJ/mol	Joback Method
hvap	38.72	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.055		Crippen Method
mcvol	108.830	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	479.31	K	Joback Method
tc	698.65	K	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=R283637&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature