Heptane, 1-isothiocyanato-

Other names:	n-Heptyl isothiocyanate
	Heptyl isothiocyanate
Inchi:	InChI=1S/C8H15NS/c1-2-3-4-5-6-7-9-8-10/h2-7H2,1H3
InchiKey:	LIPUQNPCPLDDBO-UHFFFAOYSA-N
Formula:	C8H15NS
SMILES:	CCCCCCCN=C=S
Mol. weight [g/mol]:	157.28
CAS:	4426-83-9

Physical Properties

Property code	Value	Unit	Source
hf	75.62	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.060		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1228.90		NIST Webbook
rinpol	1264.40		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1228.90		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	528.39	K	Joback Method
tc	736.35	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4426839&Units=SI
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

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