Octane, 1-isothiocyanato-

Other names:	Isothiocyanic acid, octyl ester
	n-Octyl isothiocyanate
	Octyl isothiocyanate
Inchi:	InChI=1S/C9H17NS/c1-2-3-4-5-6-7-8-10-9-11/h2-8H2,1H3
InchiKey:	YEZHGQZHWKJPCM-UHFFFAOYSA-N
Formula:	C9H17NS
SMILES:	CCCCCCCCN=C=S
Mol. weight [g/mol]:	171.30
CAS:	4430-45-9

Physical Properties

Property code	Value	Unit	Source
hf	54.98	kJ/mol	Joback Method
hvap	46.07	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.450		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1367.60		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1367.60		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook
tb	551.27	K	Joback Method
tc	756.06	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=C4430459&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature