

Undecyl isothiocyanate

Inchi:	InChI=1S/C12H23NS/c1-2-3-4-5-6-7-8-9-10-11-13-12-14/h2-11H2,1H3
InchiKey:	CFGGVVRPLBWNDW-UHFFFAOYSA-N
Formula:	C12H23NS
SMILES:	CCCCCCCCCCCCN=C=S
Mol. weight [g/mol]:	213.38
CAS:	19010-96-9

Physical Properties

Property code	Value	Unit	Source
hf	-6.94	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.620		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
tb	619.91	K	Joback Method
tc	816.21	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=C19010969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/39-015-2/Undecyl-isothiocyanate.pdf>

Generated by Cheméo on 2025-12-20 03:57:42.413051391 +0000 UTC m=+5951259.943092056.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.