t-Octyl isothiocyanate

Other names:	1,1,3,3-tetramethylbutyl isothiocyanate
	tert-Octyl isothiocyanate
Inchi:	InChI=1S/C9H17NS/c1-8(2,3)6-9(4,5)10-7-11/h6H2,1-5H3
InchiKey:	KUGHMFIBHMZICO-UHFFFAOYSA-N
Formula:	C9H17NS
SMILES:	CC(C)(C)CC(C)(C)N=C=S
Mol. weight [g/mol]:	171.31

Physical Properties

Property code	Value	Unit	Source
hf	-32.02	kJ/mol	Cheméo Relay (1.0)
hvap	51.87	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
logp	3.304		Crippen Method
mcvol	155.400	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C17701767&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume