Hexadecyl isothiocyanate

Inchi:	InChI=1S/C17H33NS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-17-19/h2-16H2,1H3
InchiKey:	KLULJVSOVKADRQ-UHFFFAOYSA-N
Formula:	C17H33NS
SMILES:	CCCCCCCCCCCCCCCCN=C=S
Mol. weight [g/mol]:	283.52
CAS:	4426-87-3

Physical Properties

Property code	Value	Unit	Source
hf	-110.14	kJ/mol	Joback Method
hvap	63.88	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.571		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
tb	734.31	K	Joback Method
tc	922.72	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4426873&Units=SI

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

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