2-Octane isothiocyanate

Inchi: InChI=1S/C9H17NS/c1-3-4-5-6-7-9(2)10-8-11/h9H,3-7H2,1-2H3
InchiKey: RXAAZXUXIQEORL-UHFFFAOYSA-N
Formula: C9H17NS
SMILES: CCCCCCC(C)N=C=S
Mol. weight [g/mol]: 171.30
CAS: 69626-80-8

Physical Properties

Property code	Value	Unit	Source
hf	49.70	kJ/mol	Joback Method
hvap	45.68	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.448		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
tb	550.83	K	Joback Method
tc	760.02	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=C69626808&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