Nonyl isothiocyanate

Inchi:	InChI=1S/C10H19NS/c1-2-3-4-5-6-7-8-9-11-10-12/h2-9H2,1H3
InchiKey:	GSAYWRFRZHSPQB-UHFFFAOYSA-N
Formula:	C10H19NS
SMILES:	CCCCCCCCCN=C=S
Mol. weight [g/mol]:	185.33
CAS:	4430-43-7

Physical Properties

Property code	Value	Unit	Source
hf	34.34	kJ/mol	Joback Method
hvap	48.29	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.840		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1458.00		NIST Webbook
ripol	1862.00		NIST Webbook
tb	574.15	K	Joback Method
tc	775.91	K	Joback Method

Sources

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=C4430437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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