n-Pentyl isothiocyanate

Other names:	Pentyl isothiocyanate
	n-Amyl isothiocyanate
	Pentane, 1-isothiocyanato-
Inchi:	InChI=1S/C6H11NS/c1-2-3-4-5-7-6-8/h2-5H2,1H3
InchiKey:	SGHJUJBYMSVAJY-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	CCCCCN=C=S
Mol. weight [g/mol]:	129.22
CAS:	629-12-9

Physical Properties

Property code	Value	Unit	Source
hf	116.90	kJ/mol	Joback Method
hvap	39.39	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.279		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1079.40		NIST Webbook
rinpol	1079.40		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1077.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	482.63	K	Joback Method
tc	697.10	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=C629129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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