

Propane, 1-isothiocyanato-

Other names:	Isothiocyanic acid, propyl ester n-Propyl isothiocyanate Propyl isothiocyanate Isothiocyanic acid n-propyl ester
Inchi:	InChI=1S/C4H7NS/c1-2-3-5-4-6/h2-3H2,1H3
InchiKey:	KKASGUHLXWAKEZ-UHFFFAOYSA-N
Formula:	C4H7NS
SMILES:	CCCN=C=S
Mol. weight [g/mol]:	101.17
CAS:	628-30-8

Physical Properties

Property code	Value	Unit	Source
hf	158.18	kJ/mol	Joback Method
hvap	34.94	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.499		Crippen Method
mvol	84.950	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rmpol	880.90		NIST Webbook
rmpol	880.90		NIST Webbook
tb	436.87	K	Joback Method
tc	657.70	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C628308&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{inpol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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