Allyl Isothiocyanate

Other names:	1-Propene, 3-isothiocyanato-
	2-Propenyl isothiocyanate
	3-Isothiocyanato-1-propene
	3-iso-Thiocyanatoprop-1-ene
	AITC
	Allyl isosulfocyanate
	Allyl mustard oil
	Allyl thioisocyanate
	Allylsenevol
	Allylsenfoel
	Allylsevenolum
	Allyspol
	Allyspol 75EC
	Carbospol
	Isothiocyanate d'allyle
	Isothiocyanic acid, allyl ester
	Mustard oil
	NCI-C50464
	NSC 5572
	Oil of mustard
	Oil of mustard, artificial
	Oleum sinapis
	Oleum sinapis volatile
	Propene, 3-isothiocyanato-
	Redskin
	Senfoel
	Synthetic mustard oil
	Volatile mustard oil
	Volatile oil of mustard
Inchi:	InChI=1S/C4H5NS/c1-2-3-5-4-6/h2H,1,3H2
InchiKey:	ZOJBYZNEUISWFT-UHFFFAOYSA-N
Formula:	C4H5NS
SMILES:	C=CCN=C=S
Mol. weight [g/mol]:	99.15
CAS:	57-06-7

Physical Properties

Property code	Value	Unit	Source
hf	283.61	kJ/mol	Joback Method
hvap	42.10	kJ/mol	NIST Webbook
log10ws	-1.28		Crippen Method
logp	1.275		Crippen Method
mcvol	80.650	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
rinpol	882.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	860.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1356.00		NIST Webbook
tb	425.05 ± 0.30	K	NIST Webbook
tb	421.35 ± 1.50	K	NIST Webbook
tb	434.15 ± 0.50	K	NIST Webbook
tc	659.61	K	Joback Method
tf	173.15 ± 1.50	K	NIST Webbook
tf	170.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	156.90	J/mol×K	290.00	NIST Webbook
hvapt	47.60	kJ/mol	300.00	NIST Webbook
hvapt	56.80	kJ/mol	400.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33108e+01
Coeff. B	-3.00384e+03
Coeff. C	-7.95820e+01
Temperature range (K), min.	310.23
Temperature range (K), max.	455.09

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1865.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57067&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpl: Liquid phase heat capacity

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point