Benzene, (isothiocyanatomethyl)-

Other names:	AB 2
	Benzyl Isothiocyanate
	Benzyl mustard oil
	Benzylsenfoel
	Isothiocyanic acid, benzyl ester
	NSC 118976
	Toluene, «alpha»-isothiocyanato-
	Toluene, Â«alphaÂ»-isothiocyanato-
	Tromacaps
	Tromalyt
	Urogran
Inchi:	InChI=1S/C8H7NS/c10-7-9-6-8-4-2-1-3-5-8/h1-5H,6H2
InchiKey:	MDKCFLQDBWCQCV-UHFFFAOYSA-N
Formula:	C8H7NS
SMILES:	S=C=NCc1ccccc1
Mol. weight [g/mol]:	149.21
CAS:	622-78-6

Physical Properties

Property code	Value	Unit	Source
hf	312.15	kJ/mol	Joback Method
hvap	46.12	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.289		Crippen Method
mcvol	117.550	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1377.90		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1377.90		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1391.00		NIST Webbook

rinpol	1389.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1317.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2071.00		NIST Webbook
tb	516.00	K	NIST Webbook
tc	814.89	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	62.20	kJ/mol	434.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.50 ± 0.50	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.81400e+01
Coeff. B	-6.77895e+03
Coeff. C	-1.48100e+01

Temperature range (K), min.	352.00
Temperature range (K), max.	543.24

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=C622786&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature