

Benzene, isothiocyanato-

Other names:	Benzene-1-isothiocyanate Fenylisothiokyanat Isothiocyanatobenzene Isothiocyanic acid, phenyl ester NSC 5583 PITC Phenyl isothiocyanate Phenyl mustard oil Phenyl thioisocyanate Phenylsenfoel Thiocarbanil USAF M-4
Inchi:	InChI=1S/C7H5NS/c9-6-8-7-4-2-1-3-5-7/h1-5H
InchiKey:	QKFJKGMPGYROCL-UHFFFAOYSA-N
Formula:	C7H5NS
SMILES:	S=C=Nc1ccccc1
Mol. weight [g/mol]:	135.19
CAS:	103-72-0

Physical Properties

Property code	Value	Unit	Source
chl	-4289.00	kJ/mol	NIST Webbook
chl	-4286.10	kJ/mol	NIST Webbook
hf	332.79	kJ/mol	Joback Method
hfl	212.00	kJ/mol	NIST Webbook
hvap	43.89	kJ/mol	Joback Method
ie	8.52 ± 0.01	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.421		Crippen Method
mcvol	103.460	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
tb	491.65 ± 2.00	K	NIST Webbook
tb	494.15 ± 1.00	K	NIST Webbook
tc	798.03	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	186.20	J/mol×K	290.00	NIST Webbook
hvapt	52.60	kJ/mol	406.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35559e+01
Coeff. B	-3.71471e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	352.55
Temperature range (K), max.	529.09

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103720&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions

hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/25-631-3/Benzene-isothiocyanato.pdf>

Generated by Cheméo on 2024-04-27 08:04:44.110027809 +0000 UTC m=+16494333.030605133.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.