

Thiocyanic acid, phenyl ester

Other names:	Phenyl thiocyanate Phenylrhodanid
Inchi:	InChI=1S/C7H5NS/c8-6-9-7-4-2-1-3-5-7/h1-5H
InchiKey:	YXCDJKQYFBEAOU-UHFFFAOYSA-N
Formula:	C7H5NS
SMILES:	N#CSc1ccccc1
Mol. weight [g/mol]:	135.19
CAS:	5285-87-0

Physical Properties

Property code	Value	Unit	Source
chl	-4340.52	kJ/mol	NIST Webbook
gf	286.77	kJ/mol	Joback Method
hf	255.47	kJ/mol	Joback Method
hfl	267.00	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.260		Crippen Method
mcvol	103.460	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	557.10	K	Joback Method
tc	815.58	K	Joback Method
tf	294.46	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.03	J/mol×K	557.10	Joback Method
cpg	210.35	J/mol×K	600.18	Joback Method
cpg	218.92	J/mol×K	643.26	Joback Method
cpg	226.76	J/mol×K	686.34	Joback Method
cpg	233.92	J/mol×K	729.42	Joback Method

cpg	240.41	J/mol×K	772.50	Joback Method
cpg	246.28	J/mol×K	815.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.20	K	0.10	NIST Webbook

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=C5285870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/61-542-2/Thiocyanic-acid-phenyl-ester.pdf>

Generated by Cheméo on 2025-12-06 03:42:00.689466873 +0000 UTC m=+4740718.219507539.

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