

1-allyl-3-phenyl-2-thiourea

Other names:	N-Allyl-N'-phenylthiourea Allylphenylthiourea
Inchi:	InChI=1S/C10H12N2S/c1-2-8-11-10(13)12-9-6-4-3-5-7-9/h2-7H,1,8H2,(H2,11,12,13)
InchiKey:	RJTICPGQFMYYEG-UHFFFAOYSA-N
Formula:	C10H12N2S
SMILES:	C=CCNC(=S)Nc1ccccc1
Mol. weight [g/mol]:	192.28
CAS:	7341-63-1

Physical Properties

Property code	Value	Unit	Source
gf	529.41	kJ/mol	Joback Method
hf	365.67	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.159		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	621.94	K	Joback Method
tc	856.78	K	Joback Method
tf	375.00 ± 1.00	K	NIST Webbook
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.85	J/mol×K	739.36	Joback Method
cpg	410.84	J/mol×K	778.50	Joback Method
cpg	420.13	J/mol×K	817.64	Joback Method
cpg	365.57	J/mol×K	621.94	Joback Method
cpg	378.31	J/mol×K	661.08	Joback Method
cpg	390.04	J/mol×K	700.22	Joback Method
cpg	428.79	J/mol×K	856.78	Joback Method

cps	59.00	J/mol×K	323.00	NIST Webbook
hfust	27.61	kJ/mol	375.00	NIST Webbook
sfust	73.60	J/mol×K	375.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27177328&Units=SI
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

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/58-736-1/1-allyl-3-phenyl-2-thiourea.pdf>

Generated by Cheméo on 2025-12-05 17:17:39.118176023 +0000 UTC m=+4703256.648216677.

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