

2-propyl-2-thiazoline

Other names:	Thiazole, 4,5-dihydro-2-propyl
Inchi:	InChI=1S/C6H11NS/c1-2-3-6-7-4-5-8-6/h2-5H2,1H3
InchiKey:	FOHLKSYCRUXPJC-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	CCCC1=NCCS1
Mol. weight [g/mol]:	129.22

Physical Properties

Property code	Value	Unit	Source
gf	220.87	kJ/mol	Joback Method
hf	76.19	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.932		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1442.00		NIST Webbook
tb	462.30	K	Joback Method
tc	692.18	K	Joback Method
tf	340.79	K	Joback Method
vc	0.395	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.81	J/mol×K	462.30	Joback Method
cpg	233.86	J/mol×K	500.61	Joback Method
cpg	247.12	J/mol×K	538.93	Joback Method

cpg	259.61	J/mol×K	577.24	Joback Method
cpg	271.36	J/mol×K	615.56	Joback Method
cpg	282.39	J/mol×K	653.87	Joback Method
cpg	292.71	J/mol×K	692.18	Joback Method

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=R88247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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/92-351-0/2-propyl-2-thiazoline.pdf>

Generated by Cheméo on 2024-04-20 08:50:07.953545837 +0000 UTC m=+15892256.874123234.

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