

5-ethyl-2-octyl-3-thiazoline

Inchi:	InChI=1S/C13H25NS/c1-3-5-6-7-8-9-10-13-14-11-12(4-2)15-13/h11-13H,3-10H2,1-2H3
InchiKey:	HWOQPDRUEFXJEK-UHFFFAOYSA-N
Formula:	C13H25NS
SMILES:	CCCCCCCC1N=CC(CC)S1
Mol. weight [g/mol]:	227.41

Physical Properties

Property code	Value	Unit	Source
gf	274.02	kJ/mol	Joback Method
hf	-97.50	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	56.79	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.659		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinsol	1765.00		NIST Webbook
tb	608.14	K	Joback Method
tc	811.77	K	Joback Method
tf	398.68	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.74	J/mol×K	608.14	Joback Method
cpg	576.22	J/mol×K	642.08	Joback Method
cpg	595.59	J/mol×K	676.02	Joback Method
cpg	613.88	J/mol×K	709.95	Joback Method
cpg	631.11	J/mol×K	743.89	Joback Method
cpg	647.31	J/mol×K	777.83	Joback Method
cpg	662.50	J/mol×K	811.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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