

5-ethyl-2-hexyl-4-methyl-3-thiazoline, trans

Inchi:	InChI=1S/C12H23NS/c1-4-6-7-8-9-12-13-10(3)11(5-2)14-12/h11-12H,4-9H2,1-3H3/t11-,14
InchiKey:	DFOVDUGPGMCNJO-RYUDHWPXSA-N
Formula:	C12H23NS
SMILES:	CCCCCCC1N=C(C)C(CC)S1
Mol. weight [g/mol]:	213.38

Physical Properties

Property code	Value	Unit	Source
gf	255.97	kJ/mol	Joback Method
hf	-88.33	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.269		Crippen Method
mvol	191.110	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	1947.00		NIST Webbook
tb	590.24	K	Joback Method
tc	797.96	K	Joback Method
tf	399.93	K	Joback Method
vc	0.729	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.26	J/molxK	590.24	Joback Method
cpg	523.09	J/molxK	624.86	Joback Method
cpg	541.88	J/molxK	659.48	Joback Method
cpg	559.65	J/molxK	694.10	Joback Method
cpg	576.42	J/molxK	728.72	Joback Method
cpg	592.19	J/molxK	763.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498205&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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