

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

Inchi:	InChI=1S/C13H25NS/c1-4-6-7-8-9-10-13-14-11(3)12(5-2)15-13/h12-13H,4-10H2,1-3H3/t
InchiKey:	NECBSIDGPQBUKF-STQMWFEESA-N
Formula:	C13H25NS
SMILES:	CCCCCCCC1N=C(C)C(CC)S1
Mol. weight [g/mol]:	227.41

Physical Properties

Property code	Value	Unit	Source
gf	264.39	kJ/mol	Joback Method
hf	-108.97	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	57.46	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.659		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1702.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2068.00		NIST Webbook
tb	613.12	K	Joback Method
tc	817.68	K	Joback Method
tf	411.20	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.11	J/mol×K	613.12	Joback Method
cpg	576.35	J/mol×K	647.21	Joback Method
cpg	595.53	J/mol×K	681.31	Joback Method
cpg	613.65	J/mol×K	715.40	Joback Method

cpg	630.75	J/mol×K	749.49	Joback Method
cpg	646.83	J/mol×K	783.59	Joback Method
cpg	661.92	J/mol×K	817.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498161&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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