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

Inchi: InChI=1S/C13H25NS/c1-4-6-7-8-9-10-13-14-12(5-2)11(3)15-13/h11,13H,4-10H2,1-3H3/t
InchiKey: VHLVMEQNZOXCMH-AAEUAGOBSA-N
Formula: C13H25NS
SMILES: CCCCCCCC1N=C(CC)C(C)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	1691.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1691.00		NIST Webbook
ripol	2030.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497866&Units=SI

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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