5-ethyl-2-pentyl-3-thiazoline

Inchi: InChI=1S/C10H19NS/c1-3-5-6-7-10-11-8-9(4-2)12-10/h8-10H,3-7H2,1-2H3
InchiKey: CGOHUCILTZWZDW-UHFFFAOYSA-N
Formula: C10H19NS
SMILES: CCCCCC1N=CC(CC)S1
Mol. weight [g/mol]: 185.33

Physical Properties

Property code	Value	Unit	Source
gf	248.76	kJ/mol	Joback Method
hf	-35.58	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.489		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1443.00		NIST Webbook
tb	539.50	K	Joback Method
tc	753.02	K	Joback Method
tf	364.87	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.71	J/mol×K	539.50	Joback Method
cpg	420.72	J/mol×K	575.09	Joback Method
cpg	438.73	J/mol×K	610.67	Joback Method
cpg	455.73	J/mol×K	646.26	Joback Method
cpg	471.77	J/mol×K	681.85	Joback Method
cpg	486.84	J/mol×K	717.44	Joback Method
cpg	500.98	J/mol×K	753.02	Joback Method

Sources

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=R498270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume