2-pentyl-4-methyl-3-thiazoline

Inchi: InChI=1S/C9H17NS/c1-3-4-5-6-9-10-8(2)7-11-9/h9H,3-7H2,1-2H3
InchiKey: RBIUXEMZVMJJOG-UHFFFAOYSA-N
Formula: C9H17NS
SMILES: CCCCCC1N=C(C)CS1
Mol. weight [g/mol]: 171.31

Physical Properties

Property code	Value	Unit	Source
hfus	22.63	kJ/mol	Joback Method
logp	3.101		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
rinpol	1377.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1377.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1804.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.32	J/mol×K	526.27	Joback Method
cpg	370.83	J/mol×K	562.67	Joback Method
cpg	387.41	J/mol×K	599.07	Joback Method
cpg	403.07	J/mol×K	635.47	Joback Method
cpg	417.84	J/mol×K	671.87	Joback Method
cpg	431.73	J/mol×K	708.27	Joback Method
cpg	444.77	J/mol×K	744.67	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498121&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices