4-methyl-2-pentyl-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]: 171.30

Physical Properties

Property code	Value	Unit	Source
gf	238.42	kJ/mol	Joback Method
hf	-6.07	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.101		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2811.36	kPa	Joback 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
tb	526.27	K	Joback Method
tc	744.67	K	Joback Method
tf	370.36	K	Joback Method
vc	0.561	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498121&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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