2-Isobutyl-4,5-dimethyl-3-thiazoline

Inchi: InChI=1S/C9H17NS/c1-6(2)5-9-10-7(3)8(4)11-9/h6,8-9H,5H2,1-4H3
InchiKey: FDOISHJOXPONIV-UHFFFAOYSA-N
Formula: C9H17NS
SMILES: CC1=NC(CC(C)C)SC1C
Mol. weight [g/mol]: 171.31

Physical Properties

Property code	Value	Unit	Source
hfus	20.18	kJ/mol	Joback Method
logp	2.955		Crippen Method
mcvol	148.840	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.44	J/mol×K	521.16	Joback Method
cpg	372.87	J/mol×K	558.38	Joback Method
cpg	390.33	J/mol×K	595.59	Joback Method
cpg	406.83	J/mol×K	632.81	Joback Method
cpg	422.40	J/mol×K	670.03	Joback Method
cpg	437.03	J/mol×K	707.25	Joback Method
cpg	450.73	J/mol×K	744.46	Joback Method

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R230821&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume