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]: 171.30

Physical Properties

Property code	Value	Unit	Source
gf	228.27	kJ/mol	Joback Method
hf	-31.69	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.955		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1240.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1241.00		NIST Webbook
tb	521.16	K	Joback Method
tc	744.46	K	Joback Method
tf	351.12	K	Joback Method
vc	0.554	m3/kmol	Joback 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R230821&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume