2-butyl-4,5-dimethyl-3-thiazoline, cis

Inchi: InChI=1S/C9H17NS/c1-4-5-6-9-10-7(2)8(3)11-9/h8-9H,4-6H2,1-3H3/t8-,9+/m1/s1
InchiKey: AZBKKBJOXUCAPP-BDAKNGLRSA-N
Formula: C9H17NS
SMILES: CCCCC1N=C(C)C(C)S1
Mol. weight [g/mol]: 171.30

Physical Properties

Property code	Value	Unit	Source
gf	230.71	kJ/mol	Joback Method
hf	-26.41	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.099		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	521.60	K	Joback Method
tc	739.88	K	Joback Method
tf	366.12	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.20	J/mol×K	521.60	Joback Method
cpg	372.14	J/mol×K	557.98	Joback Method
cpg	389.16	J/mol×K	594.36	Joback Method
cpg	405.29	J/mol×K	630.74	Joback Method

cpg	420.52	J/mol×K	667.12	Joback Method
cpg	434.87	J/mol×K	703.50	Joback Method
cpg	448.35	J/mol×K	739.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497420&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

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