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

Inchi: InChI=1S/C9H17NS/c1-4-5-6-9-10-7(2)8(3)11-9/h8-9H,4-6H2,1-3H3/t8-,9-/m0/s1
InchiKey: AZBKKBJOXUCAPP-IUCAKERBSA-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	1308.00		NIST Webbook
rinpol	1303.00		NIST Webbook
ripol	1683.00		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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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