2-butyl-5-methyl-3-thiazoline, cis

Inchi: InChI=1S/C8H15NS/c1-3-4-5-8-9-6-7(2)10-8/h6-8H,3-5H2,1-2H3/t7-,8+/m1/s1
InchiKey: FSRWQOGXZZHFMJ-SFYZADRCSA-N
Formula: C8H15NS
SMILES: CCCCC1N=CC(C)S1
Mol. weight [g/mol]: 157.28

Physical Properties

Property code	Value	Unit	Source
gf	231.92	kJ/mol	Joback Method
hf	5.70	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Joback Method
hvap	45.66	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.709		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1237.00		NIST Webbook
tb	493.74	K	Joback Method
tc	714.46	K	Joback Method
tf	342.33	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.40	J/mol×K	493.74	Joback Method
cpg	324.84	J/mol×K	530.53	Joback Method
cpg	341.36	J/mol×K	567.31	Joback Method
cpg	356.97	J/mol×K	604.10	Joback Method
cpg	371.70	J/mol×K	640.89	Joback Method
cpg	385.55	J/mol×K	677.68	Joback Method
cpg	398.55	J/mol×K	714.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497564&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