2-butyl-4-methyl-3-thiazoline

Inchi: InChI=1S/C8H15NS/c1-3-4-5-8-9-7(2)6-10-8/h8H,3-6H2,1-2H3
InchiKey: FQYKDIIJARQCAP-UHFFFAOYSA-N
Formula: C8H15NS
SMILES: CCCCC1N=C(C)CS1
Mol. weight [g/mol]: 157.28

Physical Properties

Property code	Value	Unit	Source
gf	230.00	kJ/mol	Joback Method
hf	14.57	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	46.63	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.710		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1272.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	503.39	K	Joback Method
tc	725.54	K	Joback Method
tf	359.09	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.19	J/mol×K	503.39	Joback Method
cpg	323.82	J/mol×K	540.41	Joback Method
cpg	339.57	J/mol×K	577.44	Joback Method
cpg	354.46	J/mol×K	614.46	Joback Method
cpg	368.50	J/mol×K	651.49	Joback Method
cpg	381.70	J/mol×K	688.51	Joback Method

cpg	394.10	J/mol×K	725.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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