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

Inchi: InChI=1S/C8H15NS/c1-5(2)8-9-6(3)7(4)10-8/h5,7-8H,1-4H3/t7-,8-/m0/s1
InchiKey: FVCWUBASYJVIEJ-YUMQZZPRSA-N
Formula: C8H15NS
SMILES: CC1=NC(C(C)C)SC1C
Mol. weight [g/mol]: 157.28

Physical Properties

Property code	Value	Unit	Source
gf	219.85	kJ/mol	Joback Method
hf	-11.05	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	45.94	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.565		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1518.00		NIST Webbook
tb	498.28	K	Joback Method
tc	725.54	K	Joback Method
tf	339.85	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.24	J/mol×K	498.28	Joback Method
cpg	325.76	J/mol×K	536.16	Joback Method
cpg	342.38	J/mol×K	574.03	Joback Method
cpg	358.10	J/mol×K	611.91	Joback Method
cpg	372.93	J/mol×K	649.78	Joback Method
cpg	386.88	J/mol×K	687.66	Joback Method
cpg	399.95	J/mol×K	725.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497742&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume