

5-ethyl-2-isobutyl-4-methyl-3-thiazoline, trans

Inchi:	InChI=1S/C10H19NS/c1-5-9-8(4)11-10(12-9)6-7(2)3/h7,9-10H,5-6H2,1-4H3/t9-,10-/m0/s
InchiKey:	KQXISUWXTVZWVG-UWVGGRQHSA-N
Formula:	C10H19NS
SMILES:	CCC1SC(CC(C)C)N=C1C
Mol. weight [g/mol]:	185.33

Physical Properties

Property code	Value	Unit	Source
gf	236.69	kJ/mol	Joback Method
hf	-52.33	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.345		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1349.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	544.04	K	Joback Method
tc	763.45	K	Joback Method
tf	362.39	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.48	J/mol×K	544.04	Joback Method
cpg	421.65	J/mol×K	580.61	Joback Method
cpg	439.81	J/mol×K	617.18	Joback Method
cpg	456.98	J/mol×K	653.75	Joback Method
cpg	473.15	J/mol×K	690.31	Joback Method

cpg	488.34	J/mol×K	726.88	Joback Method
cpg	502.58	J/mol×K	763.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498245&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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