2-hexyl-4-methyl-3-thiazoline

Inchi: InChI=1S/C10H19NS/c1-3-4-5-6-7-10-11-9(2)8-12-10/h10H,3-8H2,1-2H3
InchiKey: JPTKVCPJBACSLI-UHFFFAOYSA-N
Formula: C10H19NS
SMILES: CCCCCCC1N=C(C)CS1
Mol. weight [g/mol]: 185.33

Physical Properties

Property code	Value	Unit	Source
gf	246.84	kJ/mol	Joback Method
hf	-26.71	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.491		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	1915.00		NIST Webbook
tb	549.15	K	Joback Method
tc	763.88	K	Joback Method
tf	381.63	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.26	J/mol×K	549.15	Joback Method
cpg	419.51	J/mol×K	584.94	Joback Method
cpg	436.78	J/mol×K	620.73	Joback Method
cpg	453.10	J/mol×K	656.51	Joback Method
cpg	468.48	J/mol×K	692.30	Joback Method
cpg	482.95	J/mol×K	728.09	Joback Method
cpg	496.52	J/mol×K	763.88	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=R497460&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