2-heptyl-4-methyl-3-thiazoline

Inchi: InChI=1S/C11H21NS/c1-3-4-5-6-7-8-11-12-10(2)9-13-11/h11H,3-9H2,1-2H3
InchiKey: CRWZGRLIGQCFCP-UHFFFAOYSA-N
Formula: C11H21NS
SMILES: CCCCCCCC1N=C(C)CS1
Mol. weight [g/mol]: 199.36

Physical Properties

Property code	Value	Unit	Source
gf	255.26	kJ/mol	Joback Method
hf	-47.35	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.881		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1589.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
tb	572.03	K	Joback Method
tc	783.21	K	Joback Method
tf	392.90	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.90	J/mol×K	572.03	Joback Method
cpg	469.76	J/mol×K	607.23	Joback Method
cpg	487.61	J/mol×K	642.42	Joback Method
cpg	504.47	J/mol×K	677.62	Joback Method
cpg	520.36	J/mol×K	712.81	Joback Method

cpg	535.31	J/mol×K	748.01	Joback Method
cpg	549.33	J/mol×K	783.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497455&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

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