2-pentyl-4-ethyl-3-thiazoline

Inchi: InChI=1S/C10H19NS/c1-3-5-6-7-10-11-9(4-2)8-12-10/h10H,3-8H2,1-2H3
InchiKey: KPARJFOWMANKBG-UHFFFAOYSA-N
Formula: C10H19NS
SMILES: CCCCCC1N=C(CC)CS1
Mol. weight [g/mol]: 185.34

Physical Properties

Property code	Value	Unit	Source
hfus	25.22	kJ/mol	Joback Method
logp	3.491		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
rinpol	1457.00		NIST Webbook
rinpol	1453.00		NIST Webbook
ripol	1847.00		NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R497995&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices