4-ethyl-2-heptyl-3-thiazoline

Inchi: InChI=1S/C12H23NS/c1-3-5-6-7-8-9-12-13-11(4-2)10-14-12/h12H,3-10H2,1-2H3
InchiKey: OKFHLKBNWQXEJK-UHFFFAOYSA-N
Formula: C12H23NS
SMILES: CCCCCCCC1N=C(CC)CS1
Mol. weight [g/mol]: 213.38

Physical Properties

Property code	Value	Unit	Source
gf	263.68	kJ/mol	Joback Method
hf	-67.99	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	55.54	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.271		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1669.00		NIST Webbook
ripol	2064.00		NIST Webbook
tb	594.91	K	Joback Method
tc	802.71	K	Joback Method
tf	404.17	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.14	J/mol×K	594.91	Joback Method
cpg	521.50	J/mol×K	629.54	Joback Method
cpg	539.82	J/mol×K	664.18	Joback Method
cpg	557.13	J/mol×K	698.81	Joback Method
cpg	573.43	J/mol×K	733.44	Joback Method
cpg	588.77	J/mol×K	768.08	Joback Method
cpg	603.17	J/mol×K	802.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497846&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