4,5-dimethyl-2-heptyl-3-thiazoline, trans

Inchi: InChI=1S/C12H23NS/c1-4-5-6-7-8-9-12-13-10(2)11(3)14-12/h11-12H,4-9H2,1-3H3/t11-,1
InchiKey: HXPLKOIQTIJDPL-RYUDHWBXSA-N
Formula: C12H23NS
SMILES: CCCCCCCC1N=C(C)C(C)S1
Mol. weight [g/mol]: 213.38

Physical Properties

Property code	Value	Unit	Source
gf	255.97	kJ/mol	Joback Method
hf	-88.33	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.269		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1623.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1996.00		NIST Webbook
tb	590.24	K	Joback Method
tc	797.96	K	Joback Method
tf	399.93	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.26	J/mol×K	590.24	Joback Method
cpg	523.09	J/mol×K	624.86	Joback Method
cpg	541.88	J/mol×K	659.48	Joback Method
cpg	559.65	J/mol×K	694.10	Joback Method

cpg	576.42	J/mol×K	728.72	Joback Method
cpg	592.19	J/mol×K	763.34	Joback Method
cpg	607.00	J/mol×K	797.96	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=R497668&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