2-Methyl-4-n-propyl-delta^2-thiazoline

Other names: 2-Methyl-4-n-propyl-delta
Inchi: InChI=1S/C7H13NS/c1-3-4-7-5-9-6(2)8-7/h7H,3-5H2,1-2H3
InchiKey: MLGJXLTTXXFOAD-UHFFFAOYSA-N
Formula: C7H13NS
SMILES: CCCC1CSC(C)=N1
Mol. weight [g/mol]: 143.25
CAS: 4146-20-7

Physical Properties

Property code	Value	Unit	Source
gf	221.58	kJ/mol	Joback Method
hf	35.21	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	44.41	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.320		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	480.51	K	Joback Method
tc	706.42	K	Joback Method
tf	347.82	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.96	J/mol×K	480.51	Joback Method
cpg	278.56	J/mol×K	518.16	Joback Method
cpg	293.34	J/mol×K	555.81	Joback Method
cpg	307.32	J/mol×K	593.47	Joback Method
cpg	320.50	J/mol×K	631.12	Joback Method
cpg	332.91	J/mol×K	668.77	Joback Method
cpg	344.55	J/mol×K	706.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4146207&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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