

2,5-Dimethyl-delta²-thiazoline

Other names:	2,5-Dimethyl-delta
Inchi:	InChI=1S/C5H9NS/c1-4-3-6-5(2)7-4/h4H,3H2,1-2H3
InchiKey:	QURBTAPQPXENJD-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CC1=NCC(C)S1
Mol. weight [g/mol]:	115.20
CAS:	4146-19-4

Physical Properties

Property code	Value	Unit	Source
gf	204.74	kJ/mol	Joback Method
hf	76.49	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	39.96	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.540		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	434.75	K	Joback Method
tc	667.99	K	Joback Method
tf	325.28	K	Joback Method
vc	0.338	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.71	J/molxK	434.75	Joback Method
cpg	193.73	J/molxK	473.62	Joback Method
cpg	206.08	J/molxK	512.50	Joback Method
cpg	217.78	J/molxK	551.37	Joback Method
cpg	228.84	J/molxK	590.24	Joback Method
cpg	239.24	J/molxK	629.12	Joback Method
cpg	249.02	J/molxK	667.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4146194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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