

2,5-Dihydrothiazole, 2,4,5-trimethyl

Inchi:	InChI=1S/C6H11NS/c1-4-5(2)8-6(3)7-4/h5-6H,1-3H3
InchiKey:	AIVVNNYXOSPRCW-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	CC1=NC(C)SC1C
Mol. weight [g/mol]:	129.22

Physical Properties

Property code	Value	Unit	Source
gf	205.45	kJ/mol	Joback Method
hf	35.51	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.929		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	452.96	K	Joback Method
tc	682.33	K	Joback Method
tf	332.31	K	Joback Method
vc	0.393	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.65	J/mol×K	452.96	Joback Method
cpg	236.39	J/mol×K	491.19	Joback Method
cpg	250.42	J/mol×K	529.42	Joback Method
cpg	263.75	J/mol×K	567.64	Joback Method
cpg	276.38	J/mol×K	605.87	Joback Method
cpg	288.31	J/mol×K	644.10	Joback Method
cpg	299.53	J/mol×K	682.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R643915&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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