2H-Tetrazole, 2,5-dimethyl-

Inchi: InChI=1S/C3H6N4/c1-3-4-6-7(2)5-3/h1-2H3
InchiKey: HVRBCXZGTURXBT-UHFFFAOYSA-N
Formula: C3H6N4
SMILES: Cc1nnn(C)n1
Mol. weight [g/mol]: 98.11
CAS: 4135-93-7

Physical Properties

Property code	Value	Unit	Source
chs	-2240.50 ± 2.80	kJ/mol	NIST Webbook
hf	251.20 ± 2.90	kJ/mol	NIST Webbook
hfs	202.50 ± 2.90	kJ/mol	NIST Webbook
hsub	48.70 ± 0.50	kJ/mol	NIST Webbook
hsub	48.70	kJ/mol	NIST Webbook
log10ws	-2.53		Crippen Method
logp	-0.481		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
tt	257.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	13.50	kJ/mol	256.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4135937&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature