3,5-Dimethyl-1H-1,2,4-triazole

Inchi: InChI=1S/C4H7N3/c1-3-5-4(2)7-6-3/h1-2H3,(H,5,6,7)
InchiKey: XYYXDARQOHWBPO-UHFFFAOYSA-N
Formula: C4H7N3
SMILES: Cc1n[nH]c(C)n1
Mol. weight [g/mol]: 97.12

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	Cheméo Relay (1.0)
logp	-0.060		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
tb	531.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.20	K	2.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7343342&Units=SI

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure