1,2,4-Triazine

Other names: as-Triazine
Inchi: InChI=1S/C3H3N3/c1-2-5-6-3-4-1/h1-3H
InchiKey: FYADHXFMURLYQI-UHFFFAOYSA-N
Formula: C3H3N3
SMILES: c1cnncn1
Mol. weight [g/mol]: 81.08
CAS: 290-38-0

Physical Properties

Property code	Value	Unit	Source
ie	9.20	eV	NIST Webbook
ie	9.61	eV	NIST Webbook
log10ws	-0.77		Crippen Method
logp	-0.128		Crippen Method
mcvol	59.310	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.20	K	98.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C290380&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure