1,3,3-Trinitropiperidine

Other names:	1,4,4-Trinitropiperidine
Inchi:	InChI=1S/C5H8N4O6/c10-7(11)5(8(12)13)1-3-6(4-2-5)9(14)15/h1-4H2
InchiKey:	HOVMRGMHBFQKOI-UHFFFAOYSA-N
Formula:	C5H8N4O6
SMILES:	O=[N+]([O-])N1CCC([N+](=O)[O-])([N+](=O)[O-])CC1
Mol. weight [g/mol]:	220.14
CAS:	298228-66-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	-0.476		Crippen Method
mcvol	132.690	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	100.40	kJ/mol	389.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C298228667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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https://www.chemeo.com/cid/98-408-1/1-3-3-Trinitropiperidine.pdf

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