1,3-Dinitro-1,3-diazacycloheptane

Inchi: InChI=1S/C5H10N4O4/c10-8(11)6-3-1-2-4-7(5-6)9(12)13/h1-5H2
InchiKey: XFBIFYVTPFYRSQ-UHFFFAOYSA-N
Formula: C5H10N4O4
SMILES: O=[N+]([O-])N1CCCCN([N+](=O)[O-])C1
Mol. weight [g/mol]: 190.16
CAS: 5754-90-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	-0.275		Crippen Method
mcvol	125.250	ml/mol	McGowan Method
tf	374.00 ± 0.10	K	NIST Webbook
tf	376.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	2.80	kJ/mol	374.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5754905&Units=SI

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
tf:	Normal melting (fusion) point