

3,5,7-Trioxa-1,1,1,9,9,9-hexanitrononane

Inchi:	InChI=1S/C6H8N6O15/c13-7(14)5(8(15)16,9(17)18)1-25-3-27-4-26-2-6(10(19)20,11(21)22)
InchiKey:	YLDAILBJBDQTQG-UHFFFAOYSA-N
Formula:	C6H12N6O15
SMILES:	O=[N+](O-)[C](COCOCOCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	408.19
CAS:	80308-91-4

Physical Properties

Property code	Value	Unit	Source
chs	-2907.50 ± 0.80	kJ/mol	NIST Webbook
gf	-96.38	kJ/mol	Joback Method
hf	-645.89	kJ/mol	Joback Method
hfs	-597.10 ± 1.20	kJ/mol	NIST Webbook
hfus	68.20	kJ/mol	Joback Method
hvap	133.13	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	-2.081		Crippen Method
mcvol	217.530	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	1308.52	K	Joback Method
tc	1614.94	K	Joback Method
tf	1090.57	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.17	J/mol×K	1308.52	Joback Method
cpg	682.51	J/mol×K	1359.59	Joback Method
cpg	681.13	J/mol×K	1410.66	Joback Method
cpg	679.16	J/mol×K	1461.73	Joback Method
cpg	676.73	J/mol×K	1512.80	Joback Method
cpg	673.96	J/mol×K	1563.87	Joback Method
cpg	670.97	J/mol×K	1614.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80308914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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