

1,3,5-Triazine, 2,4,6-trimethoxy-

Other names:	s-Triazine, 2,4,6-trimethoxy- Trimethyl cyanurate 2,4,6-Trimethoxy-s-triazine 2,4,6-Trimethoxy-1,3,5-triazine 2,4,6-Trimethoxy-[1,3,5]-triazin
Inchi:	InChI=1S/C6H9N3O3/c1-10-4-7-5(11-2)9-6(8-4)12-3/h1-3H3
InchiKey:	DFUGJTBMQKRCPI-UHFFFAOYSA-N
Formula:	C6H9N3O3
SMILES:	COc1nc(OC)nc(OC)n1
Mol. weight [g/mol]:	171.15
CAS:	877-89-4

Physical Properties

Property code	Value	Unit	Source
chs	-3169.04 ± 0.82	kJ/mol	NIST Webbook
chs	-3168.69 ± 0.83	kJ/mol	NIST Webbook
hf	-387.90 ± 1.50	kJ/mol	NIST Webbook
hfs	-478.30 ± 1.20	kJ/mol	NIST Webbook
hfs	-478.60 ± 0.87	kJ/mol	NIST Webbook
hsub	90.33 ± 0.94	kJ/mol	NIST Webbook
hsub	88.20 ± 1.30	kJ/mol	NIST Webbook
hsub	90.30 ± 1.00	kJ/mol	NIST Webbook
hsub	88.20 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.13		Crippen Method
logp	-0.103		Crippen Method
mcpvol	119.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	207.00	J/mol×K	298.15	NIST Webbook
hfust	18.10	kJ/mol	410.50	NIST Webbook
hsubt	90.33	kJ/mol	298.15	NIST Webbook
hsubt	86.60 ± 1.30	kJ/mol	338.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C877894&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ssubt:	Entropy of sublimation at a given temperature

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