Triazintrione, 1,3,5-triphenyl-

Other names: s-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-triphenyl-
Phenyl isocyanate trimer
Phenyl isocyanurate
Triphenyl isocyanurate
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-triphenyl-
1,3,5-Triphenyl-1,3,5-perhydro-triazine-2,4,6-trione
1,3,5-Triphenyl-perhydro-1,3,5-triazine-2,4,6-trione
1,3,5-Triphenyl-s-triazine-2,4,6-trione
1,3,5-Triphenyl-1,3,5-triazine-2,4,6-trione
Phenyl isocyanate cyclic trimer
1,3,5-Triphenyl-2,4,6-triazinetrione
s-Triazine-2,4,6(1H,3H,5H)-trione, triphenyl-
1,3,5-Triphenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
Triazintrione, 1,3,5-triphenyl-
1,3,5-Triphenyl isocyanurate
N,N',N''-Triphenyl isocyanurate
NSC 105886
NSC 82068

Inchi: InChI=1S/C21H15N3O3/c25-19-22(16-10-4-1-5-11-16)20(26)24(18-14-8-3-9-15-18)21(27
InchiKey: YEACGXMAEGBJSM-UHFFFAOYSA-N
Formula: C21H15N3O3
SMILES: O=c1n(-c2ccccc2)c(=O)n(-c2ccccc2)c(=O)n1-c1ccccc1
Mol. weight [g/mol]: 357.37

Physical Properties

Property code	Value	Unit	Source
chs	-10063.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-344.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-344.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.25	eV	Cheméo Relay (1.0)
logp	2.139		Crippen Method
mcvol	259.260	ml/mol	McGowan Method
tf	502.83	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1785020&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point