

STYPHNIC ACID

Other names:	1,3-Benzenediol, 2,4,6-trinitro-Styphnic acid Resorcinol, 2,4,6-trinitro-2,4-Dihydroxy-1,3,5-trinitrobenzene 2,4,6-Trinitro-1,3-benzenediol 1,3-Dihydroxy-2,4,6-trinitrobenzene 3-Hydroxy-2,4,6-trinitrophenol NSC 36932
Inchi:	InChI=1S/C6H3N3O8/c10-5-2(7(12)13)1-3(8(14)15)6(11)4(5)9(16)17/h1,10-11H
InchiKey:	IXHMHWIBCIYOAZ-UHFFFAOYSA-N
Formula:	C6H3N3O8
SMILES:	O=[N+](O-)[c1cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c1O
Mol. weight [g/mol]:	245.10

Physical Properties

Property code	Value	Unit	Source
chs	-2322.30 ± 6.90	kJ/mol	NIST Webbook
chs	-2246.89	kJ/mol	NIST Webbook
chs	-2356.90	kJ/mol	NIST Webbook
hf	-226.62	kJ/mol	Cheméo Relay (1.0)
hfs	-542.92	kJ/mol	NIST Webbook
hfs	-467.50 ± 6.90	kJ/mol	NIST Webbook
hfs	-433.00	kJ/mol	NIST Webbook
hfus	50.21	kJ/mol	Joback Method
hsub	120.80 ± 1.10	kJ/mol	NIST Webbook
hvap	84.97	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-3.16		Cheméo Relay (1.0)
logp	0.822		Crippen Method
mcvol	135.640	ml/mol	McGowan Method
tb	529.45	K	Cheméo Relay (1.0)
tf	454.90 ± 0.40	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.10	J/mol×K	990.08	Joback Method
cpg	394.99	J/mol×K	1040.27	Joback Method
cpg	404.78	J/mol×K	1090.47	Joback Method
cpg	415.76	J/mol×K	1140.66	Joback Method
cpg	428.20	J/mol×K	1190.86	Joback Method
cpg	442.37	J/mol×K	1241.05	Joback Method
cpg	458.55	J/mol×K	1291.24	Joback Method
hfust	33.50	kJ/mol	454.90	NIST Webbook
hfust	33.50	kJ/mol	454.80	NIST Webbook
hfust	33.50	kJ/mol	454.80	NIST Webbook
sfust	73.60	J/mol×K	454.90	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82713&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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