2,4,6,-Trinitro-1,3,5,-tris(methylnitramino)benzene

Inchi: InChI=1S/C9H9N9O12/c1-10(16(25)26)4-7(13(19)20)5(11(2)17(27)28)9(15(23)24)6(8(4)
InchiKey: HHROXJLCXHZPFK-UHFFFAOYSA-N
Formula: C9H9N9O12
SMILES: CN(c1c([N+](=O)[O-])c(N(C)[N+](=O)[O-])c([N+](=O)[O-])c(N(C)[N+](=O)[O-])c1[N+](=O)[
Mol. weight [g/mol]: 435.22
CAS: 62030-37-9

Physical Properties

Property code	Value	Unit	Source
chs	-4945.90 ± 9.60	kJ/mol	NIST Webbook
gf	634.80	kJ/mol	Joback Method
hf	88.12	kJ/mol	Joback Method
hfs	118.10 ± 9.60	kJ/mol	NIST Webbook
hfus	88.39	kJ/mol	Joback Method
hvap	146.89	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	0.295		Crippen Method
mcvol	248.370	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	1405.26	K	Joback Method
tc	1724.07	K	Joback Method
tf	1239.28	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.17	J/mol×K	1405.26	Joback Method
cpg	792.12	J/mol×K	1458.39	Joback Method
cpg	796.23	J/mol×K	1511.53	Joback Method
cpg	800.69	J/mol×K	1564.66	Joback Method
cpg	805.72	J/mol×K	1617.80	Joback Method
cpg	811.52	J/mol×K	1670.93	Joback Method
cpg	818.29	J/mol×K	1724.07	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62030379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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