1,1,4,4-Tetranitrocyclohexane

Inchi:	InChI=1S/C6H8N4O8/c11-7(12)5(8(13)14)1-2-6(4-3-5,9(15)16)10(17)18/h1-4H2
InchiKey:	ZOLAMORIQWZYQZ-UHFFFAOYSA-N
Formula:	C6H8N4O8
SMILES:	O=[N+]([O-])C1([N+](=O)[O-])CCC([N+](=O)[O-])([N+](=O)[O-])CC1
Mol. weight [g/mol]:	264.15
CAS:	146028-82-2

Physical Properties

Property code	Value	Unit	Source
gf	147.60	kJ/mol	Joback Method
hf	-145.75	kJ/mol	Joback Method
hfus	37.05	kJ/mol	Joback Method
hvap	93.13	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	0.060		Crippen Method
mcvol	154.220	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	959.40	K	Joback Method
tc	1279.93	K	Joback Method
tf	782.76	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.16	J/mol×K	959.40	Joback Method
cpg	525.23	J/mol×K	1012.82	Joback Method
cpg	547.98	J/mol×K	1066.24	Joback Method
cpg	574.08	J/mol×K	1119.67	Joback Method
cpg	604.18	J/mol×K	1173.09	Joback Method
cpg	638.94	J/mol×K	1226.51	Joback Method
cpg	679.01	J/mol×K	1279.93	Joback Method
hfust	108.80	kJ/mol	489.20	NIST Webbook

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=C146028822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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