Naphthalene, 1,3,6,8-tetranitro-

Other names: 1,3,6,8-Tetranitronaphthalene
Inchi: InChI=1S/C10H4N4O8/c15-11(16)6-1-5-2-7(12(17)18)4-9(14(21)22)10(5)8(3-6)13(19)20/
InchiKey: BFMBQYIQQLBGJA-UHFFFAOYSA-N
Formula: C10H4N4O8
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2c1
Mol. weight [g/mol]: 308.16
CAS: 28995-89-3

Physical Properties

Property code	Value	Unit	Source
gf	356.06	kJ/mol	Joback Method
hf	88.95	kJ/mol	Joback Method
hfus	56.60	kJ/mol	Joback Method
hvap	110.78	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	2.473		Crippen Method
mcvol	178.220	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	442.85		NIST Webbook
rinpol	442.85		NIST Webbook
tb	1101.14	K	Joback Method
tc	1409.82	K	Joback Method
tf	886.10	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.06	J/mol×K	1101.14	Joback Method
cpg	518.05	J/mol×K	1152.59	Joback Method
cpg	523.72	J/mol×K	1204.03	Joback Method
cpg	529.21	J/mol×K	1255.48	Joback Method
cpg	534.69	J/mol×K	1306.93	Joback Method
cpg	540.30	J/mol×K	1358.38	Joback Method

cpg	546.23	J/mol×K	1409.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28995893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume