Diphenyl ether, 2,4,6-trinitro-

Other names: 1,3,5-trinitro-2-phenoxy-benzene
Inchi: InChI=1S/C12H7N3O7/c16-13(17)8-6-10(14(18)19)12(11(7-8)15(20)21)22-9-4-2-1-3-5-9/
InchiKey: KDVCTAHYZJQAOH-UHFFFAOYSA-N
Formula: C12H7N3O7
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(Oc2ccccc2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 305.20
CAS: 6973-40-6

Physical Properties

Property code	Value	Unit	Source
gf	247.74	kJ/mol	Joback Method
hf	-16.86	kJ/mol	Joback Method
hfus	49.02	kJ/mol	Joback Method
hvap	101.03	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.203		Crippen Method
mcvol	190.550	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	1020.20	K	Joback Method
tc	1317.25	K	Joback Method
tf	768.46	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.38	J/mol×K	1020.20	Joback Method
cpg	558.65	J/mol×K	1069.71	Joback Method
cpg	563.69	J/mol×K	1119.22	Joback Method
cpg	567.56	J/mol×K	1168.72	Joback Method
cpg	570.35	J/mol×K	1218.23	Joback Method
cpg	572.15	J/mol×K	1267.74	Joback Method
cpg	573.03	J/mol×K	1317.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6973406&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume