1,4-Dinitrocyclooctatetraene

Inchi: InChI=1S/C8H6N2O4/c11-9(12)7-3-1-2-4-8(6-5-7)10(13)14/h1-6H/b2-1-,3-1-,4-2-,6-5-,7-
InchiKey: GRMYFWFBOIJSEI-REXIGCOJSA-N
Formula: C8H6N2O4
SMILES: O=[N+]([O-])C1=CC=C([N+](=O)[O-])C=CC=C1
Mol. weight [g/mol]: 194.14
CAS: 54755-18-9

Physical Properties

Property code	Value	Unit	Source
gf	196.12	kJ/mol	Joback Method
hf	40.55	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	70.16	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	1.434		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	725.48	K	Joback Method
tc	1013.06	K	Joback Method
tf	499.80	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.40	J/mol×K	725.48	Joback Method
cpg	340.17	J/mol×K	773.41	Joback Method
cpg	349.71	J/mol×K	821.34	Joback Method
cpg	358.07	J/mol×K	869.27	Joback Method
cpg	365.29	J/mol×K	917.20	Joback Method
cpg	371.42	J/mol×K	965.13	Joback Method
cpg	376.49	J/mol×K	1013.06	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=C54755189&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
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