2,4-Dinitrophenylmethylnitramine

Inchi: InChI=1S/C7H6N4O6/c1-8(11(16)17)6-3-2-5(9(12)13)4-7(6)10(14)15/h2-4H,1H3
InchiKey: BUGRLMJGTJHURD-UHFFFAOYSA-N
Formula: C7H6N4O6
SMILES: CN(c1ccc([N+](=O)[O-])cc1[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 242.15
CAS: 19092-03-6

Physical Properties

Property code	Value	Unit	Source
chs	-3628.20 ± 3.70	kJ/mol	NIST Webbook
gf	318.64	kJ/mol	Joback Method
hf	61.03	kJ/mol	Joback Method
hfs	16.20 ± 3.70	kJ/mol	NIST Webbook
hfus	44.25	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	1.131		Crippen Method
mcvol	147.970	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	864.16	K	Joback Method
tc	1147.85	K	Joback Method
tf	683.41	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.43	J/mol×K	864.16	Joback Method
cpg	420.28	J/mol×K	911.44	Joback Method
cpg	427.21	J/mol×K	958.72	Joback Method
cpg	433.31	J/mol×K	1006.01	Joback Method
cpg	438.67	J/mol×K	1053.29	Joback Method
cpg	443.38	J/mol×K	1100.57	Joback Method
cpg	447.54	J/mol×K	1147.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19092036&Units=SI

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