2,4-Dinitrobenzaldehyde

Other names: Benzaldehyde, 2,4-dinitro-
Inchi: InChI=1S/C7H4N2O5/c10-4-5-1-2-6(8(11)12)3-7(5)9(13)14/h1-4H
InchiKey: ZILXIZUBLXVYPI-UHFFFAOYSA-N
Formula: C7H4N2O5
SMILES: O=Cc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 196.12
CAS: 528-75-6

Physical Properties

Property code	Value	Unit	Source
gf	72.79	kJ/mol	Joback Method
hf	-81.32	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Calorimetric study and thermal analysis of crystalline 2,4-dinitrobenzaldehyde (C7H4N2O5)
hvap	74.68	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	1.315		Crippen Method
mcvol	122.140	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	748.54	K	Joback Method
tc	1021.37	K	Joback Method
tf	549.33	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.20	J/mol×K	748.54	Joback Method
cpg	313.09	J/mol×K	794.01	Joback Method
cpg	320.14	J/mol×K	839.48	Joback Method
cpg	326.41	J/mol×K	884.95	Joback Method
cpg	331.94	J/mol×K	930.43	Joback Method

cpg	336.79	J/mol×K	975.90	Joback Method
cpg	341.00	J/mol×K	1021.37	Joback Method
hfust	21.18	kJ/mol	223.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.20	K	1.30	NIST Webbook

Sources

Calorimetric study and thermal analysis of crystalline 2,4-dinitrobenzaldehyde (C7H4N2O5):	https://www.doi.org/10.1016/j.jct.2004.09.018
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=C528756&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume