

2,4-Dinitrobenzoic acid

Other names:	Benzoic acid, 2,4-dinitro-
Inchi:	InChI=1S/C7H4N2O6/c10-7(11)5-2-1-4(8(12)13)3-6(5)9(14)15/h1-3H,(H,10,11)
InchiKey:	ZIIGSRYPZWDGBT-UHFFFAOYSA-N
Formula:	C7H4N2O6
SMILES:	O=C(O)c1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	212.12
CAS:	610-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-93.43	kJ/mol	Joback Method
hf	-260.55	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hsub	135.00 ± 2.00	kJ/mol	NIST Webbook
hvap	91.38	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.201		Crippen Method
mcvol	128.010	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	845.93	K	Joback Method
tc	1098.09	K	Joback Method
tf	618.08	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.23	J/mol×K	972.01	Joback Method
cpg	357.31	J/mol×K	1014.04	Joback Method
cpg	360.85	J/mol×K	1056.06	Joback Method
cpg	337.32	J/mol×K	845.93	Joback Method
cpg	343.27	J/mol×K	887.96	Joback Method
cpg	348.56	J/mol×K	929.98	Joback Method
cpg	363.88	J/mol×K	1098.09	Joback Method

hfust	30.60	kJ/mol	455.80	NIST Webbook
hsubt	132.00 ± 2.00	kJ/mol	383.00	NIST Webbook
hvapt	92.00 ± 3.00	kJ/mol	523.50	NIST Webbook
hvapt	91.00 ± 1.00	kJ/mol	516.50	NIST Webbook

Sources

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=C610300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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