

Dinitro-2,6-phenol

Other names:	o-Dinitrophenol Phenol, «beta»-dinitro- 2,6-Dinitrophenol «beta»-Dinitrophenol 2,6-Dinitrofenol Dinitro-2,6-phenol
Inchi:	InChI=1S/C6H4N2O5/c9-6-4(7(10)11)2-1-3-5(6)8(12)13/h1-3,9H
InchiKey:	JCRIDWXIBSEOEK-UHFFFAOYSA-N
Formula:	C6H4N2O5
SMILES:	O=[N+]([O-])c1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	184.11

Physical Properties

Property code	Value	Unit	Source
chs	-2722.80 ± 2.70	kJ/mol	NIST Webbook
chs	-2723.10 ± 3.20	kJ/mol	NIST Webbook
hf	-108.00	kJ/mol	Cheméo Relay (1.0)
hfs	-209.60 ± 3.30	kJ/mol	NIST Webbook
hfus	33.45	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-2.61		Cheméo Relay (1.0)
logp	1.209		Crippen Method
mcvol	112.350	ml/mol	McGowan Method
tb	523.76	K	Cheméo Relay (1.0)
tf	385.00 ± 3.00	K	NIST Webbook
tf	336.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.88	J/mol×K	943.31	Joback Method
cpg	302.18	J/mol×K	847.98	Joback Method
cpg	327.23	J/mol×K	1038.65	Joback Method

cpg	308.65	J/mol×K	895.64	Joback Method
cpg	295.32	J/mol×K	800.31	Joback Method
cpg	287.91	J/mol×K	752.64	Joback Method
cpg	321.02	J/mol×K	990.98	Joback Method
hfust	22.91	kJ/mol	329.00	NIST Webbook
hfust	19.58	kJ/mol	336.00	NIST Webbook
hfust	19.58	kJ/mol	336.00	NIST Webbook
hfust	19.58	kJ/mol	336.00	NIST Webbook
hsubt	112.10 ± 4.20	kJ/mol	313.00	NIST Webbook
hsubt	112.10 ± 4.20	kJ/mol	293.00	NIST Webbook
hsubt	112.10 ± 4.20	kJ/mol	313.00	NIST Webbook
sfust	58.26	J/mol×K	336.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C573568&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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