Hydantoin

Other names:	2,4(3H,5H)-Imidazoledione
	2,4-Imidazolidinedione
	2-Imidazolin-4(or 5)-one, 2-hydroxy-
	Glycolylurea
	Imidazole-2,4(3H,5H)-dione
Inchi:	InChI=1S/C3H4N2O2/c6-2-1-4-3(7)5-2/h1H2,(H2,4,5,6,7)
InchiKey:	WJRBRSLFGCUECM-UHFFFAOYSA-N
Formula:	C3H4N2O2
SMILES:	O=C1CNC(=O)N1
Mol. weight [g/mol]:	100.08
CAS:	461-72-3

Physical Properties

Property code	Value	Unit	Source
chs	-1170.30 ± 0.76	kJ/mol	NIST Webbook
gf	-51.12	kJ/mol	Joback Method
hf	-224.21	kJ/mol	Joback Method
hfs	-581.90 ± 1.10	kJ/mol	NIST Webbook
hfus	14.59	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
ie	10.20 ± 0.05	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-0.40		Estimated Solubility Method
log10ws	-0.40		Aqueous Solubility Prediction Method
logp	-1.174		Crippen Method
mcvol	65.370	ml/mol	McGowan Method
pc	7267.82	kPa	Joback Method
tb	520.73	K	Joback Method
tc	783.12	K	Joback Method
tf	495.80	K	Experimental and computational study of the energetics of hydantoin and 2-thiohydantoin
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.47	J/mol×K	739.39	Joback Method
cpg	133.61	J/mol×K	520.73	Joback Method
cpg	143.17	J/mol×K	564.46	Joback Method
cpg	152.54	J/mol×K	608.19	Joback Method
cpg	161.61	J/mol×K	651.93	Joback Method
cpg	170.29	J/mol×K	695.66	Joback Method
cpg	186.06	J/mol×K	783.12	Joback Method
cps	117.09	J/mol×K	298.15	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental and computational study of the energetics of hydantoin and 2-thiohydantoin:	https://www.doi.org/10.1016/j.jct.2012.10.010
Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins:	https://www.doi.org/10.1016/j.tca.2017.06.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461723&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ie:	Ionization energy
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