4-Imidazolidinone, 2-thioxo-

Other names:	2-Thioguidanthion
	2-Thioxo-4-imidazolinone
	2-thiohydantoin
	2-thioxo-4-imidazolidinone
	Glycine thiohydantoin
	Hydantoin, 2-thio-
	Thiohydantoin
	USAF BE-25
Inchi:	InChI=1S/C3H4N2OS/c6-2-1-4-3(7)5-2/h1H2,(H2,4,5,6,7)
InchiKey:	UGWULZWUXSCWPX-UHFFFAOYSA-N
Formula:	C3H4N2OS
SMILES:	O=C1CNC(=S)N1
Mol. weight [g/mol]:	116.14
CAS:	503-87-7

Physical Properties

Property code	Value	Unit	Source
gf	162.32	kJ/mol	Joback Method
hf	28.59	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	-1.009		Crippen Method
mcvol	75.850	ml/mol	McGowan Method
pc	7640.96	kPa	Joback Method
tb	525.55	K	Joback Method
tc	792.42	K	Joback Method
tf	506.10	K	Experimental and computational study of the energetics of hydantoin and 2-thiohydantoin
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.87	J/mol×K	525.55	Joback Method
cpg	148.91	J/mol×K	570.03	Joback Method
cpg	156.55	J/mol×K	614.51	Joback Method
cpg	163.78	J/mol×K	658.99	Joback Method
cpg	170.59	J/mol×K	703.46	Joback Method
cpg	176.97	J/mol×K	747.94	Joback Method
cpg	182.89	J/mol×K	792.42	Joback Method
cps	137.05	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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C503877&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
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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