

2,4-Imidazolidinedione, 5-methyl-

Other names:	5-Methylhydantoin 5-methyl-2,4-imidazolidinedione Hydantoin, 5-methyl-
Inchi:	InChI=1S/C4H6N2O2/c1-2-3(7)6-4(8)5-2/h2H,1H3,(H2,5,6,7,8)
InchiKey:	VMAQYKGIHDWKL-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	CC1NC(=O)NC1=O
Mol. weight [g/mol]:	114.10
CAS:	616-03-5

Physical Properties

Property code	Value	Unit	Source
chs	-1944.90 ± 1.00	kJ/mol	NIST Webbook
gf	-50.41	kJ/mol	Joback Method
hf	-265.19	kJ/mol	Joback Method
hfs	-486.60 ± 1.10	kJ/mol	NIST Webbook
hfus	18.25	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	-0.786		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5899.00	kPa	Joback Method
tb	538.94	K	Joback Method
tc	795.63	K	Joback Method
tf	492.24	K	Joback Method
vc	0.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.31	J/mol×K	538.94	Joback Method
cpg	188.92	J/mol×K	581.72	Joback Method
cpg	200.21	J/mol×K	624.50	Joback Method
cpg	211.07	J/mol×K	667.28	Joback Method

cpg	221.40	J/mol×K	710.06	Joback Method
cpg	231.10	J/mol×K	752.84	Joback Method
cpg	240.07	J/mol×K	795.63	Joback Method
cps	143.11	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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
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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