Ethylphenylhydantoin

Other names:	2,4-Imidazolidinedione, 5-ethyl-5-phenyl-
	5-Ethyl-5-phenyl-2,4-imidazolidinedione
	5-Ethyl-5-phenylhydantoin
	5-Phenyl-5-ethylhydantoin
	5-ethyl-5-phenylimidazolidine-2,4-dione
	Hydantoin, 5-ethyl-5-phenyl-
	NSC 150466
	Nirvanol
	Normephenytoin
Inchi:	InChI=1S/C11H12N2O2/c1-2-11(8-6-4-3-5-7-8)9(14)12-10(15)13-11/h3-7H,2H2,1H3,(H2
InchiKey:	UDTWZFJEMMUFLC-UHFFFAOYSA-N
Formula:	C11H12N2O2
SMILES:	CCC1(c2ccccc2)NC(=O)NC1=O
Mol. weight [g/mol]:	204.23
CAS:	631-07-2

Physical Properties

Property code	Value	Unit	Source
gf	115.45	kJ/mol	Joback Method
hf	-157.90	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-2.64		Aqueous Solubility Prediction Method
logp	1.131		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1795.00		NIST Webbook
tb	726.02	K	Joback Method
tc	1004.96	K	Joback Method
tf	621.45	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.06	J/mol×K	726.02	Joback Method
cpg	447.16	J/mol×K	772.51	Joback Method
cpg	463.33	J/mol×K	819.00	Joback Method
cpg	478.69	J/mol×K	865.49	Joback Method
cpg	493.36	J/mol×K	911.98	Joback Method
cpg	507.45	J/mol×K	958.47	Joback Method
cpg	521.07	J/mol×K	1004.96	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C631072&Units=SI

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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume