

(1-Penten-2-yl) hydantoin

Inchi:	InChI=1S/C8H12N2O2/c1-3-4-5(2)6-7(11)10-8(12)9-6/h6H,2-4H2,1H3,(H2,9,10,11,12)
InchiKey:	UYGMZBYLCPNOJJ-UHFFFAOYSA-N
Formula:	C8H12N2O2
SMILES:	C=C(CCC)C1NC(=O)NC1=O
Mol. weight [g/mol]:	168.19
CAS:	116435-48-4

Physical Properties

Property code	Value	Unit	Source
gf	62.56	kJ/mol	Joback Method
hf	-232.11	kJ/mol	Joback Method
hfus	26.02	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	0.551		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	627.02	K	Joback Method
tc	871.97	K	Joback Method
tf	521.60	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.21	J/mol×K	627.02	Joback Method
cpg	356.85	J/mol×K	667.84	Joback Method
cpg	371.64	J/mol×K	708.67	Joback Method
cpg	385.52	J/mol×K	749.49	Joback Method
cpg	398.44	J/mol×K	790.32	Joback Method
cpg	410.33	J/mol×K	831.14	Joback Method
cpg	421.13	J/mol×K	871.97	Joback Method

Sources

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=C116435484&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
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

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