

(3-Methyl-1-buten-2-yl) hydantoin

Inchi:	InChI=1S/C8H12N2O2/c1-4(2)5(3)6-7(11)10-8(12)9-6/h4,6H,3H2,1-2H3,(H2,9,10,11,12)
InchiKey:	GNYHPTLIBVGYBY-UHFFFAOYSA-N
Formula:	C8H12N2O2
SMILES:	<chem>C=C(C(C)C)C1NC(=O)NC1=O</chem>
Mol. weight [g/mol]:	168.19

Physical Properties

Property code	Value	Unit	Source
gf	60.12	kJ/mol	Joback Method
hf	-237.39	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	0.407		Crippen Method
mvol	131.520	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	626.58	K	Joback Method
tc	876.99	K	Joback Method
tf	506.60	K	Joback Method
vc	0.488	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.69	J/mol×K	626.58	Joback Method
cpg	357.72	J/mol×K	668.31	Joback Method
cpg	372.85	J/mol×K	710.05	Joback Method
cpg	387.02	J/mol×K	751.78	Joback Method
cpg	400.16	J/mol×K	793.52	Joback Method
cpg	412.21	J/mol×K	835.25	Joback Method
cpg	423.09	J/mol×K	876.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003474&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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