

5-Benzylidenehydantoin

Other names:	2,4-Imidazolidinedione, 5-(phenylmethylene)-
Inchi:	InChI=1S/C10H8N2O2/c13-9-8(11-10(14)12-9)6-7-4-2-1-3-5-7/h1-6H,(H2,11,12,13,14)/b
InchiKey:	UDTSPKADQGPZFS-SOFGYWHQSA-N
Formula:	C10H8N2O2
SMILES:	O=C1NC(=O)C(=Cc2ccccc2)N1
Mol. weight [g/mol]:	188.18
CAS:	3775-01-7

Physical Properties

Property code	Value	Unit	Source
gf	165.69	kJ/mol	Joback Method
hf	-56.13	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	0.867		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	714.21	K	Joback Method
tc	997.23	K	Joback Method
tf	600.88	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.78	J/molxK	714.21	Joback Method
cpg	368.28	J/molxK	761.38	Joback Method
cpg	381.45	J/molxK	808.55	Joback Method
cpg	393.23	J/molxK	855.72	Joback Method
cpg	403.57	J/molxK	902.89	Joback Method
cpg	412.41	J/molxK	950.06	Joback Method
cpg	419.69	J/molxK	997.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3775017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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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