

Hydantoin, 5-benzylidene-2-thio-

Other names:	5-Benzylidene-2-thiohydantoin 5-Benzylidene-2-thioguidanthion 4-Imidazolidinone, 5-(phenylmethylene)-2-thioxo-
Inchi:	InChI=1S/C10H8N2OS/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:	YXMBDTHHYFCMKP-VURMDHGXSA-N
Formula:	C10H8N2OS
SMILES:	O=C1NC(=S)NC1=Cc1ccccc1
Mol. weight [g/mol]:	204.25
CAS:	583-46-0

Physical Properties

Property code	Value	Unit	Source
gf	379.13	kJ/mol	Joback Method
hf	196.67	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.032		Crippen Method
mcvol	146.420	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	719.03	K	Joback Method
tc	1005.93	K	Joback Method
tf	596.33	K	Joback Method
vc	0.531	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.46	J/mol×K	719.03	Joback Method
cpg	366.10	J/mol×K	766.85	Joback Method
cpg	377.62	J/mol×K	814.66	Joback Method
cpg	388.08	J/mol×K	862.48	Joback Method
cpg	397.53	J/mol×K	910.30	Joback Method
cpg	406.02	J/mol×K	958.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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