

2,4-Imidazolidinedione, 5-(4-methylphenyl)-5-phenyl-

Other names:

5-(p-Methylphenyl)-5-phenylhydantoin
5-Phenyl-5-(4-tolyl)hydantoin
5-(para-Methylphenyl)-5-phenylhydantoin
Hydantoin, 5-phenyl-5-(4-methylphenyl)
Hydantoin, 5-phenyl-5-(p-tolyl)
Hydantoine, 5-phenyl-5-(4-methylphenyl)
5-(4-methylphenyl)-5-phenylimidazolidine-2,4-dione

Inchi: InChI=1S/C16H14N2O2/c1-11-7-9-13(10-8-11)16(12-5-3-2-4-6-12)14(19)17-15(20)18-16

InchiKey: WPAPSGQWYNPWCZ-UHFFFAOYSA-N

Formula: C16H14N2O2

SMILES: Cc1ccc(C2(c3ccccc3)NC(=O)NC2=O)cc1

Mol. weight [g/mol]: 266.29

CAS: 51169-17-6

Physical Properties

Property code	Value	Unit	Source
gf	260.33	kJ/mol	Joback Method
hf	-36.04	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.078		Crippen Method
mvol	201.020	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	2457.00		NIST Webbook
tb	872.08	K	Joback Method
tc	1167.85	K	Joback Method
tf	716.74	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.46	J/mol×K	872.08	Joback Method

cpg	628.76	J/mol×K	921.37	Joback Method
cpg	646.09	J/mol×K	970.67	Joback Method
cpg	662.64	J/mol×K	1019.96	Joback Method
cpg	678.58	J/mol×K	1069.26	Joback Method
cpg	694.09	J/mol×K	1118.55	Joback Method
cpg	709.36	J/mol×K	1167.85	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=C51169176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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