GAMMA-PHENYL-GAMMA-BUTYROLACTONE

Other names:	«gamma»-Phenyl-«gamma»-butyrolactone
	«gamma»-Phenylbutyrolactone
	4-Phenyl-4-butanolide
	4-Phenyl-4-hydroxybutanoic acid lactone
	4-Phenylbutanolide
	4-Phenylbutyrolactone
	2(3H)-Furanone, 4,5-dihydro-5-phenyl-
	4,5-Dihydro-5-phenyl-2(3H)-furanone
	5-Phenyldihydrofuran-2(3H)-one
	NSC 24259
	NSC 48048
Inchi:	InChI=1S/C10H10O2/c11-10-7-6-9(12-10)8-4-2-1-3-5-8/h1-5,9H,6-7H2
InchiKey:	AEUULUMEYIPECD-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	O=C1CCC(c2ccccc2)O1
Mol. weight [g/mol]:	162.19

Physical Properties

Property code	Value	Unit	Source
hf	-240.94	kJ/mol	Cheméo Relay (1.0)
hfus	17.12	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	2.065		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
tb	579.20	K	NIST Webbook
tf	298.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.93	J/mol×K	564.93	Joback Method
cpg	316.66	J/mol×K	607.33	Joback Method

cpg	332.21	J/mol×K	649.73	Joback Method
cpg	346.61	J/mol×K	692.13	Joback Method
cpg	359.87	J/mol×K	734.53	Joback Method
cpg	372.03	J/mol×K	776.93	Joback Method
cpg	383.10	J/mol×K	819.33	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1008760&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point